10524956a

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NEWS 1		Web Page for STN Seminar Schedule - N. America
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NEWS 3	JAN 06	The retention policy for unread STNmail messages will change in 2009 for STN-Columbus and STN-Tokyo
NEWS 4	JAN 07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent Classification Data
NEWS 5	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 6	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 7	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS 8	FEB 10	COMPENDEX reloaded and enhanced
NEWS 9	FEB 11	WTEXTILES reloaded and enhanced
NEWS 10	FEB 19	New patent-examiner citations in 300,000 CA/CAplus patent records provide insights into related prior art
NEWS 11	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS 12	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS 13	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS 14	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS 15	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS 16	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS 17	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats
NEWS 18	MAR 11	EPFULL backfile enhanced with additional full-text applications and grants
NEWS 19	MAR 11	ESBIOBASE reloaded and enhanced
NEWS 20	MAR 20	CAS databases on STN enhanced with new super role for nanomaterial substances
NEWS 21	MAR 23	CA/CAplus enhanced with more than 250,000 patent equivalents from China
NEWS 22	MAR 30	IMSPATENTS reloaded and enhanced
NEWS 23	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS 24	APR 07	STN is raising the limits on saved answers

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 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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FILE 'HOME' ENTERED AT 14:50:04 ON 20 APR 2009

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.22       0.22

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DICTIONARY FILE UPDATES:  19 APR 2009  HIGHEST RN 1136834-47-3

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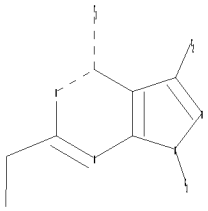
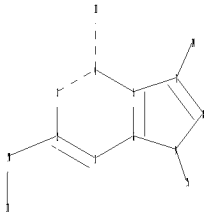




chain nodes :
10 11 14 15
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
17
chain bonds :
2-10 4-11 7-14 9-15 10-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-11 5-6 5-7 6-9 7-8 7-14 8-9 9-15
exact bonds :
2-10 10-17

G1:O,S

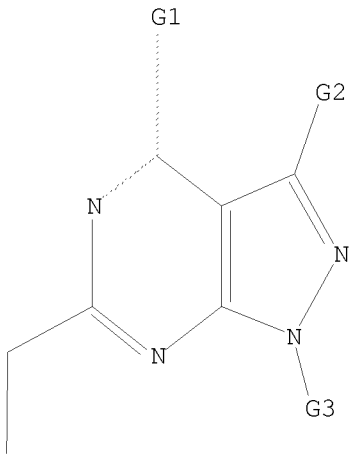
G2:H,CH3

G3:Cb,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 14:CLASS 15:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,S

G2 H,Me

G3 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 14:50:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      254 TO ITERATE

100.0% PROCESSED      254 ITERATIONS                              37 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         4124 TO     6036
PROJECTED ANSWERS:             376 TO     1104

L2           37 SEA SSS SAM L1

=> s l1 ful
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FULL SCREEN SEARCH COMPLETED -     4631 TO ITERATE

100.0% PROCESSED     4631 ITERATIONS                             625 ANSWERS
SEARCH TIME: 00.00.01

L3          625 SEA SSS FUL L1

=> fil capl
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   185.88     186.10

FILE 'CAPLUS' ENTERED AT 14:50:45 ON 20 APR 2009
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FILE COVERS 1907 - 20 Apr 2009 VOL 150 ISS 17
FILE LAST UPDATED: 19 Apr 2009 (20090419/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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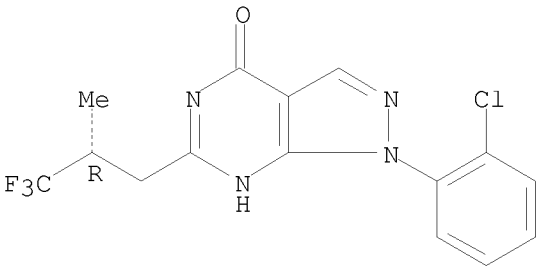
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 50 L3

=> d l4 ibib hitstr abs 1-50

L4 ANSWER 1 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1448888 CAPLUS
DOCUMENT NUMBER: 150:89649
TITLE: A Novel PDE2A Reporter Cell Line: Characterization of the Cellular Activity of PDE Inhibitors
AUTHOR(S): Wunder, Frank; Gnoth, Mark Jean; Geerts, Andreas; Barufe, Daniel
CORPORATE SOURCE: Molecular Screening Technology, Pharma Research Center, Bayer HealthCare AG, Wuppertal, D-42096, Germany
SOURCE: Molecular Pharmaceutics (2009), 6(1), 326-336
CODEN: MPOHBP; ISSN: 1543-8384
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 794568-92-6, BAY 73-6691
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(characterization of cellular activity of PDE inhibitors using novel PDE2A reporter cell line)
RN 794568-92-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.



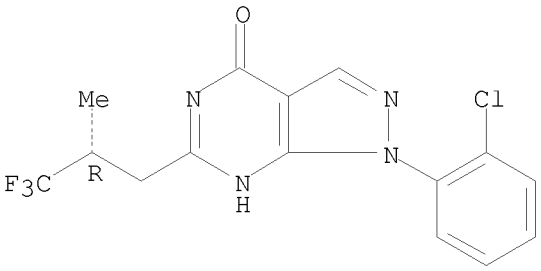
AB We report here the generation and pharmacol. characterization of a phosphodiesterase 2A (PDE2A) reporter cell line. Human PDE2A was stably transfected in a parental cell line expressing the atrial natriuretic peptide (ANP) receptor and the cyclic nucleotide-gated (CNG) cation channel CNGA2, acting as the biosensor for intracellular cGMP. In this reporter cell line, cGMP levels can be monitored in real-time via aequorin luminescence stimulated by calcium influx through the CNG channel. By using different PDE inhibitors, we could show that our PDE2A reporter assay specifically monitors PDE2A inhibition with high sensitivity. In the absence of ANP stimulation, the PDE2A selective inhibitors EHNA, BAY 60-7550 and PDP did not increase basal luminescence levels in this exptl. setting. However, in combination with ANP, these inhibitors stimulated luminescence signals and induced leftward shifts of ANP concentration-response curves. Similar results were obtained when using IBMX, trequinsin and dipyridamole, which inhibit PDE2A nonselectively with lower potency. PDP, the most potent PDE2A inhibitor known to date, was found to exhibit much lower cellular activity as anticipated from its biochem. PDE2A inhibitory activity. By cellular uptake and transport studies we could show that

PDP's cell permeability is low and that the compound is a substrate for an efflux transporter. Other PDE inhibitors including vinpocetine, milrinone, rolipram, sildenafil, zaprinast, BRL 50481 and BAY 73-6691 did not stimulate luminescence signals on our PDE2A reporter cell line. The results imply that this novel PDE2A reporter assay provides an efficient, high throughput means for the identification and characterization of PDE2A inhibitors.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1120823 CAPLUS
DOCUMENT NUMBER: 149:440143
TITLE: The novel selective PDE9 inhibitor BAY 73-6691 improves learning and memory in rodents
AUTHOR(S): van der Staay, F. Josef; Rutten, Kris; Baerfacker, Lars; DeVry, Jean; Erb, Christina; Heckroth, Heike; Karthaus, Dagmar; Tersteegen, Adrian; van Kampen, Marja; Blokland, Arjan; Prickaerts, Jos; Reymann, Klaus G.; Schroeder, Ulrich H.; Hendrix, Martin
CORPORATE SOURCE: Global Drug Discovery, Department of CNS Research, BAYER HealthCare AG, Wuppertal-Elberfeld, D-42096, Germany
SOURCE: Neuropharmacology (2008), 55(5), 908-918
CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 794568-92-6, BAY 73-6691
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel selective PDE9 inhibitor BAY 73-6691 improves learning and memory in rodents)
RN 794568-92-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.



AB The present study investigated the putative pro-cognitive effects of the novel selective PDE9 inhibitor BAY 73-6691. The effects on basal synaptic transmission and long-term potentiation (LTP) were investigated in rat hippocampal slices. Pro-cognitive effects were assessed in a series of learning and memory tasks using rodents as subjects. BAY 73-6691 had no effect on basal synaptic transmission in hippocampal slices prepared from young adult (7- to 8-wk-old) Wistar rats. A dose of 10 μM, but not 30 μM, BAY 73-6691 enhanced early LTP after weak tetanic stimulation. The dose effective in young adult Wistar rats did not affect LTP in hippocampal slices prepared from young (7- to 8-wk-old) Fischer 344 X Brown Norway (FBNF1) rats, probably reflecting strain differences. However, it increased basal synaptic transmission and enhanced early LTP after weak tetanic stimulation in hippocampal slices prepared from very old (31- to 35-mo-old) FBNF1 rats. BAY 73-6691 enhanced acquisition, consolidation, and retention of long-term memory (LTM) in a social recognition task and

tended to enhance LTM in an object recognition task. Bay 73-6691 attenuated the scopolamine-induced retention deficit in a passive avoidance task, and the MK-801-induced short-term memory deficits in a T-maze alternation task. The mechanism of action, possibly through modulation of the NO/cGMP-PKG/CREB pathway, is discussed. Our findings support the notion that PDE9 inhibition may be a novel target for treating memory deficits that are associated with aging and neurodegenerative disorders such as Alzheimer's disease.

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:256115 CAPLUS
DOCUMENT NUMBER: 148:285203
TITLE: Benzene, pyridine, and pyridazine derivatives as HSP-90 inhibitors and their preparation, pharmaceutical compositions and use in the treatment of proliferative diseases
INVENTOR(S): Huang, Kenneth He; Mangette, John; Barta, Thomas; Hughes, Philip; Hall, Steven E.; Veal, James
PATENT ASSIGNEE(S): Serenex, Inc., USA
SOURCE: PCT Int. Appl., 432pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008024978	A2	20080228	WO 2007-US76770	20070824
WO 2008024978	A3	20080821		
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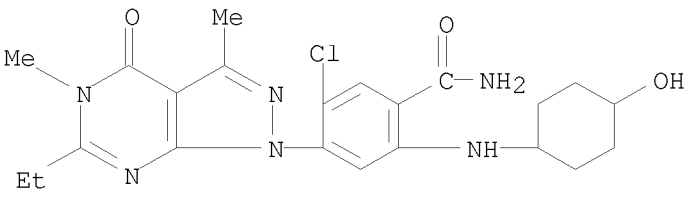
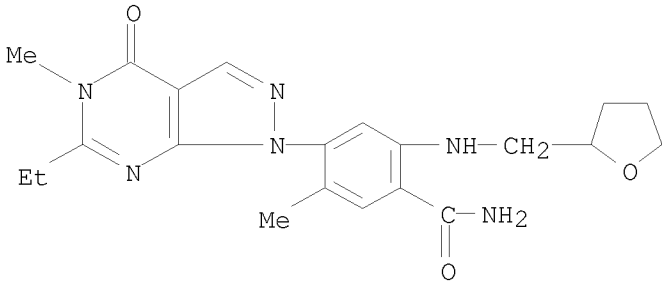
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
US 20080119457	A1	20080522	US 2007-844816	20070824

PRIORITY APPLN. INFO.: US 2006-823414P P 20060824
OTHER SOURCE(S): MARPAT 148:285203
IT 1017869-67-8P 1017872-72-8P
RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prophetic drug candidate; preparation of benzene, pyridine, and pyridazine derivs. as HSP-90 inhibitors useful in the treatment of proliferative diseases)
RN 1017869-67-8 CAPLUS
CN Benzamide, 5-chloro-4-(6-ethyl-4,5-dihydro-3,5-dimethyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-2-[(4-hydroxycyclohexyl)amino]- (CA INDEX NAME)



RN 1017872-72-8 CAPLUS
CN Benzamide, 4-(6-ethyl-4,5-dihydro-5-methyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)-5-methyl-2-[[(tetrahydro-2-furanyl)methyl]amino]- (CA INDEX NAME)



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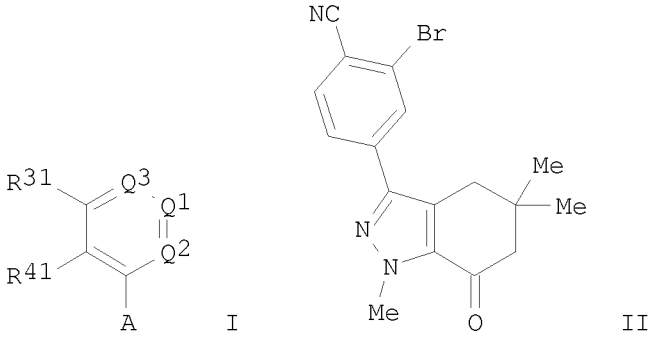

AB Disclosed are compds. and pharmaceutically acceptable salts of formula I. Compds. of formula I are useful in the treatment of diseases and/or conditions related to cell proliferation, such as cancer, inflammation, arthritis, angiogenesis, or the like. Also disclosed are pharmaceutical compns. comprising compds. of the invention and methods of treating the aforementioned conditions using such compds. Compds. of formula I wherein Q1, Q2 and Q3 are independently N and CRx, provided that no more than two of Q1, Q2 and Q3 are N; each Rx is independently H, halo, (hetero)aryl, C1-6 (halo)alkyl, etc.; A is (un)substituted (hetero)bicyclic derivative and (un)substituted 5-membered (hetero)cyclic ring; R31 and R41 are independently H, halo, C1-15 (hetero)alkyl, etc.; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by epoxidn. of 4,4-dimethylcyclohex-2-enone; the resulting 5,5-dimethyl-7-oxabicyclo[4.1.0]heptan-2-one underwent addition of methanol followed by elimination to give 2-methoxy-4,4-dimethylcyclohex-2-enone, which underwent acylation with 3-bromo-4-cyanobenzoyl chloride to give 2-bromo-4-(3-methoxy-5,5-dimethyl-2-oxocyclohex-3-enecarbonyl)benzonitrile, which underwent cyclization with methylhydrazine

to give compound II. All the invention compds. were evaluated for their HSP-90 inhibitory activity (some data given).

L4 ANSWER 4 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:729227 CAPLUS
DOCUMENT NUMBER: 147:143456
TITLE: Fused pyrimidones and thiopyrimidones, and their preparation, pharmaceutical compositions and use in killing or reducing cancer cell proliferation
INVENTOR(S): Venkat, Raj Gopal; Qi, Longwu; Pierce, Michael; Robbins, Paul B.; Sahasrabudhe, Sudhir R.; Selliah, Robert
PATENT ASSIGNEE(S): Prolexys Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 77pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007076085	A2	20070705	WO 2006-US49168	20061222
WO 2007076085	A3	20070823		

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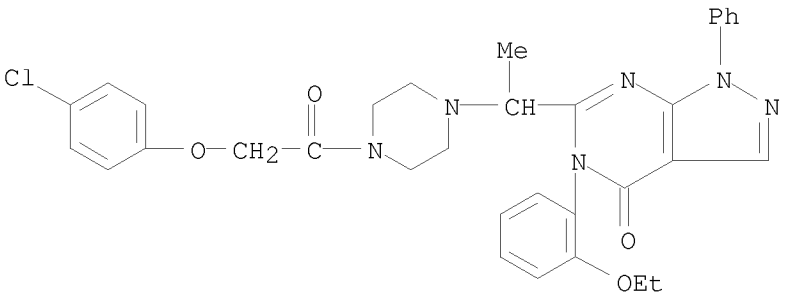
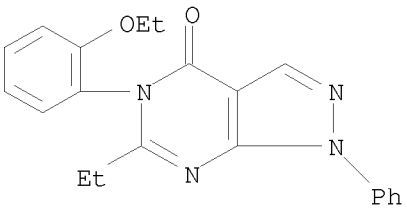
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-753916P P 20051222
US 2006-834989P P 20060727
OTHER SOURCE(S): MARPAT 147:143456
IT 943431-00-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of fused pyrimidone and thiopyrimidone compds. useful in killing or reducing cancer cell proliferation)
RN 943431-00-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[1-[4-[2-(4-chlorophenoxy)acetyl]-1-piperazinyl]ethyl]-5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl- (CA INDEX NAME)



IT 943431-16-1P 943431-17-2P 943431-18-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fused pyrimidone and thiopyrimidone compds. useful in killing or reducing cancer cell proliferation)
RN 943431-16-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(2-ethoxyphenyl)-6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



RN 943431-17-2 CAPLUS
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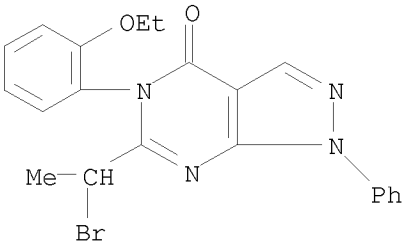
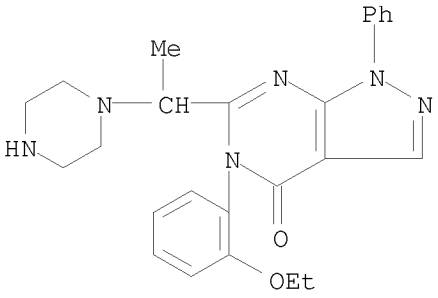


RN 943431-18-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(2-ethoxyphenyl)-1,5-dihydro-1-phenyl-6-[1-(1-piperazinyl)ethyl]- (CA INDEX NAME)



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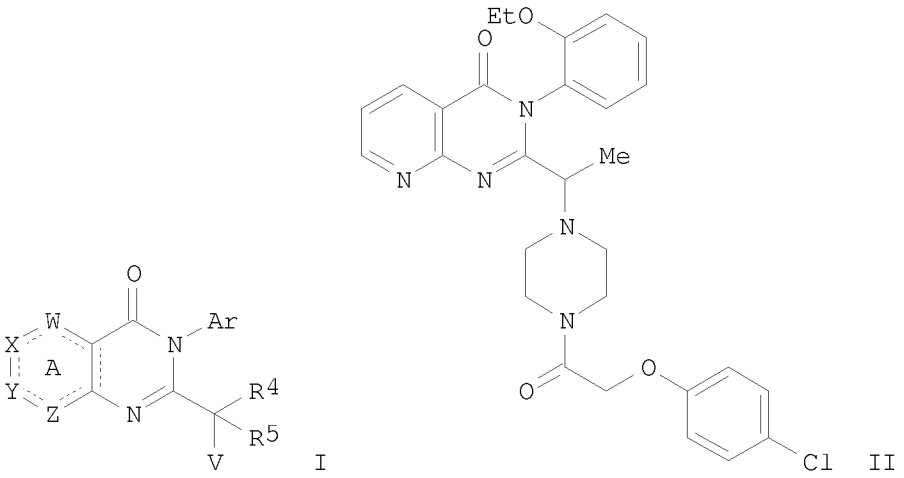
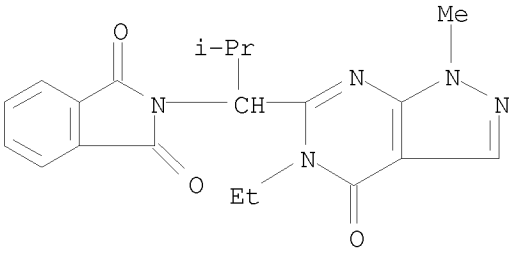


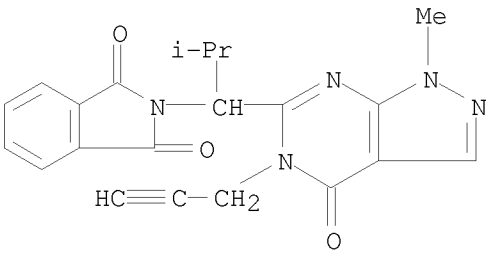
I II

AB Compds. represented by structural formula I: are useful, for example, in the effective killing or reduction in rate of proliferation of cancer cells, such as in patients suffering from cancer. In addition to the compds. themselves, the invention provides pharmaceutical compns. of the compds. and method of treatment using the compds. Compds. of formula I wherein ring A is optionally substituted: W is absent, C, N, S and O; X, Y and Z is C, N, S and O where at least one of X, Y and Z is N if W is C; Ar is (un)substituted phenyl; R4 and R5 are independently H, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted heterocyclyl, and (un)substituted aryl; V i substituted amine and cyclic amines; dotted lines are single and double bonds; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by a general procedure. All the invention compds. were evaluated for their ability to kill or reduce cancer cell proliferation.

L4 ANSWER 5 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:526013 CAPLUS
DOCUMENT NUMBER: 147:143378
TITLE: A novel synthesis of substituted 4H-pyrazolo[3,4-d]pyrimidin-4-ones
AUTHOR(S): Adams, Nicholas D.; Schmidt, Stanley J.; Knight, Steven D.; Dhanak, Dashyant
CORPORATE SOURCE: Department of Medicinal Chemistry, Microbial, Musculoskeletal, and Proliferative Diseases Centre for Excellence in Drug Discovery, GlaxoSmithKline, Collegeville, PA, 19426-0989, USA
SOURCE: Tetrahedron Letters (2007), 48(23), 3983-3986
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:143378
IT 943631-33-2P 943631-34-3P 943631-35-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of substituted pyrazolopyrimidinones from substituted amidopyrazole-carboxylates and amines via intramol. cyclization of amidines)
RN 943631-33-2 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[1-(5-ethyl-4,5-dihydro-1-methyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)-2-methylpropyl]- (CA INDEX NAME)

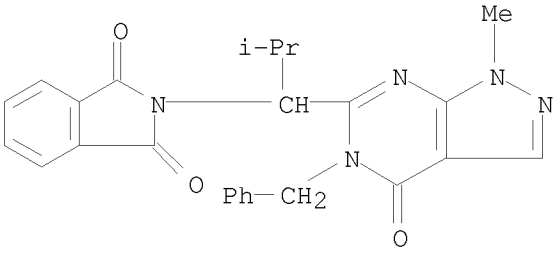


RN 943631-34-3 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[1-[4,5-dihydro-1-methyl-4-oxo-5-(2-propyn-1-yl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-2-methylpropyl]- (CA INDEX NAME)



RN 943631-35-4 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[1-[4,5-dihydro-1-methyl-4-oxo-5-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-2-methylpropyl]- (CA

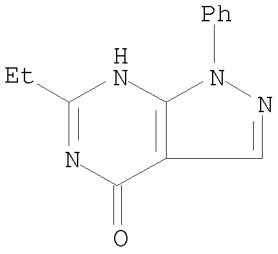
INDEX NAME)



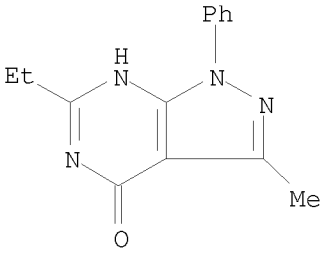
AB A novel synthesis of 4H-pyrazolo-[3,4-d]pyrimidin-4-ones is described. This approach utilizes an in situ generated iminochloride as a key precursor for amidine formation, with subsequent base-catalyzed ring closure. This method represents a mild and efficient entry into this ring system which is amenable to diversification of the core template.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:101807 CAPLUS
DOCUMENT NUMBER: 148:11168
TITLE: Synthesis of new substituted pyrazolo[3,4-d]pyrimidin-4-ones under microwave irradiation
AUTHOR(S): Davoodnia, A.; Rahimizadeh, M.; Rivadeh, Sh.; Bakavoli, M.; Roshani, M.
CORPORATE SOURCE: Department of Chemistry, School of Sciences, Islamic Azad University, Mashhad, Iran
SOURCE: Indian Journal of Heterocyclic Chemistry (2006), 16(2), 151-154
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Prof. R. S. Varma
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:11168
IT 5394-42-3P 957767-04-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of substituted pyrazolopyrimidinones by reaction of amino-phenyl-substituted-pyrazole-carboxamides with orthoesters under microwave irradiation)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



RN 957767-04-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-3-methyl-1-phenyl- (CA INDEX NAME)



AB A rapid and efficient one-pot two-component reaction of 5-amino-1-phenyl-3-substituted-1H-pyrazole-4-carboxamides and orthoesters for the synthesis of new pyrazolo[3,4-d]pyrimidin-4-one derivs. under

microwave irradiation with solid acid catalysis and under solvent-free condition is presented.

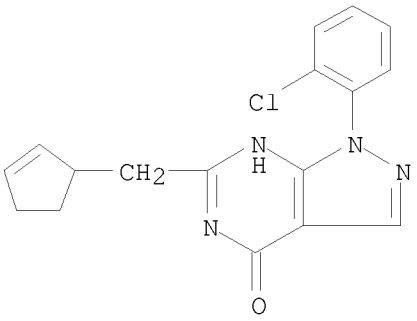
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:1253041 CAPLUS
DOCUMENT NUMBER: 146:757
TITLE: Use of pyrazolopyrimidine compounds for the treatment of cardiovascular diseases
INVENTOR(S): Hendrix, Martin; Wunder, Frank; Tersteegen, Adrian; Stasch, Johannes-Peter
PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
SOURCE: PCT Int. Appl., 48pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006125548	A1	20061130	WO 2006-EP4591	20060516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102005024493	A1	20061130	DE 2005-102005024493	20050527
EP 1888076	A1	20080220	EP 2006-753634	20060516
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: DE 2005-102005024493A 20050527
WO 2006-EP4591 W 20060516

OTHER SOURCE(S): MARPAT 146:757
IT 794568-65-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pyrazolopyrimidine compds. for treatment of cardiovascular diseases)
RN 794568-65-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX NAME)



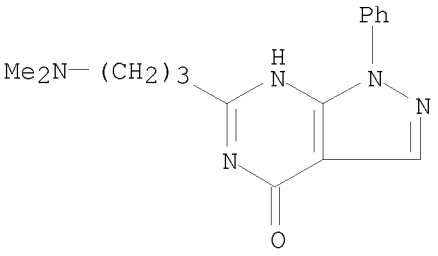
AB The invention discloses the use of pyrazolopyrimidine compds. for producing medicaments drugs for treating cardiovascular diseases.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

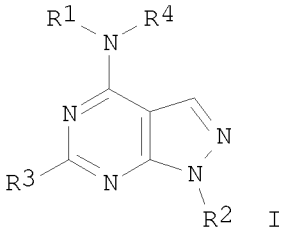
L4 ANSWER 8 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:471917 CAPLUS
DOCUMENT NUMBER: 144:488675
TITLE: Preparation of 1,4-substituted pyrazolopyrimidines as kinase inhibitors, particularly EphB4 inhibitors
INVENTOR(S): Schmiedeberg, Niko; Furet, Pascal; Imbach, Patricia; Holzer, Philipp
PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2006050946	A1	20060518	WO 2005-EP12045		20051110
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
AU 2005303965	A1	20060518	AU 2005-303965		20051110
CA 2585660	A1	20060518	CA 2005-2585660		20051110
EP 1812441	A1	20070801	EP 2005-819276		20051110
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR					
CN 101098873	A	20080102	CN 2005-80046410		20051110
JP 2008519790	T	20080612	JP 2007-540577		20051110
BR 2005017803	A	20081021	BR 2005-17803		20051110
IN 2007DN03269	A	20070831	IN 2007-DN3269		20070501
US 20080096868	A1	20080424	US 2007-718730		20070507
MX 2007005644	A	20070605	MX 2007-5644		20070510
KR 2007084191	A	20070824	KR 2007-710778		20070511
PRIORITY APPLN. INFO.:			GB 2004-25035	A	20041112
			WO 2005-EP12045	W	20051110

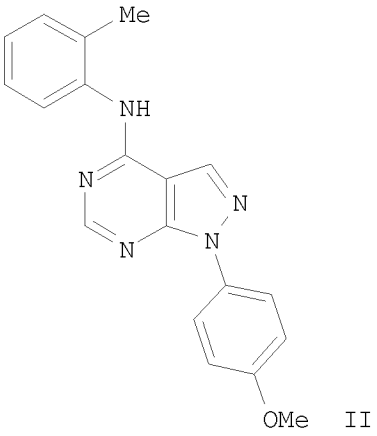
OTHER SOURCE(S): CASREACT 144:488675; MARPAT 144:488675
IT 887327-53-9P, 6-(3-Dimethylaminopropyl)-1-phenyl-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 1,4-substituted pyrazolopyrimidines as EphB4 inhibitors)
RN 887327-53-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[3-(dimethylamino)propyl]-1,5-dihydro-1-phenyl- (CA INDEX NAME)



GI



I



II

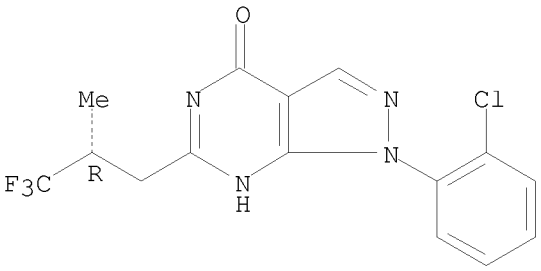
AB The invention is related to 1,4-substituted pyrazolopyrimidines I [R1 = (un)substituted Ph; R2 = (un)substituted aryl; R3 = H, (un)substituted alkyl, aryl, heterocyclyl; R4 = H, (un)substituted alkyl], and their pharmaceutically acceptable salts where one or more salt-forming groups are present, pharmaceuticals comprising them, and their use in the diagnosis and treatment or manufacture of a pharmaceutical formulation for the treatment of a disease that depends on inadequate activity of a protein kinase, especially a protein tyrosine kinase, preferably one or more of c-Abl, c-Src and/or especially Ephrin B4 receptor (EphB4) kinases; and/or one or more altered or mutated forms of any one or more of these, e.g. those forms that result in conversion of the resp. proto-oncogene into an oncogene,

such as constitutively activated Bcr-Abl or v-Src. The invention is also related to the preparation of pyrazolopyrimidines I. Thus, II•TFA was prepared starting from 4-methoxyphenylhydrazine•xHCl and (ethoxymethylene)malononitrile. Pyrazolopyrimidine II•TFA inhibited EphB4 (Ic50 = 0.16 μmol/l).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1287398 CAPLUS
DOCUMENT NUMBER: 144:100880
TITLE: Characterization of the first potent and selective PDE9 inhibitor using a cGMP reporter cell line
AUTHOR(S): Wunder, Frank; Tersteegen, Adrian; Rebmann, Annegret; Erb, Christina; Fahrig, Thomas; Hendrix, Martin
CORPORATE SOURCE: Cardiovascular Research, Bayer HealthCare AG, Wuppertal, Germany
SOURCE: Molecular Pharmacology (2005), 68(6), 1775-1781
CODEN: MOPMA3; ISSN: 0026-895X
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 794568-92-6, BAY 73-6691
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(4H-Pyrazolo[3,4-d]pyrimidin-4-one; characterization of first potent and selective PDE9 inhibitor using cGMP reporter cell line)
RN 794568-92-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]- (CA INDEX NAME)

Absolute stereochemistry.

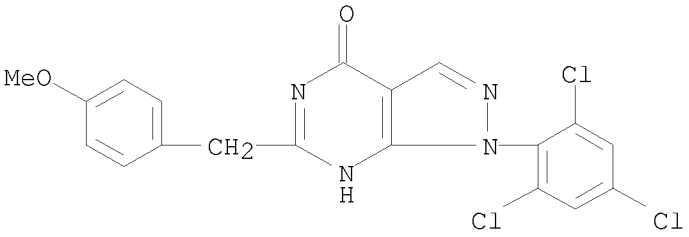


AB We report here the in vitro characterization of 1-(2-chlorophenyl)-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidine-4-one (BAY 73-6691), the first potent and selective inhibitor of phosphodiesterase 9 (PDE9), which is currently under preclin. development for the treatment of Alzheimer's disease. This compound selectively inhibits human (IC50 = 55 nM) and murine (IC50 = 100 nM) PDE9 activity in vitro and shows only moderate activity against other cyclic nucleotide-specific phosphodiesterases. We also report the generation and characterization of a stably transfected PDE9 Chinese hamster ovary cell line, addnl. expressing soluble guanylate cyclase (sGC), the olfactory cyclic nucleotide-gated cation channel CNGA2 and the photoprotein aequorin. In this cell line, intracellular cGMP levels can be monitored in real-time via aequorin luminescence induced by Ca2+ influx through CNGA2, acting as the intracellular cGMP sensor. This simple and sensitive assay system was used for the characterization of the cellular activity of the new PDE9 inhibitor. BAY 73-6691 alone did not significantly increase basal cGMP levels in this exptl. setting. However, in combination with submaximal stimulating concns. of the sGC activator

4-[((4-carboxybutyl){2-[(4-phenethylbenzyl)oxy]phenethyl}amino)methyl] benzoic acid (BAY 58-2667), the compound induced concentration-dependent luminescence signals and intracellular cGMP accumulation. The PDE9 inhibitor significantly potentiated the cGMP signals generated by sGC activating compds. such as BAY 58-2667 or 5-cyclopropyl-2-[1-(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]pyrimidin-4-ylamine (BAY 41-2272) and induced leftward shifts of the corresponding concentration-response curves. Using our newly generated PDE9 reporter cell line, we could show that BAY 73-6691 is able to efficiently penetrate cells and to inhibit intracellular PDE9 activity.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1138122 CAPLUS
DOCUMENT NUMBER: 144:100491
TITLE: A Proteome-Wide CDK/CRK-Specific Kinase Inhibitor Promotes Tumor Cell Death in the Absence of Cell Cycle Progression
AUTHOR(S): Caligiuri, Maureen; Becker, Frank; Murthi, Krishna; Kaplan, Faith; Dedier, Severine; Kaufmann, Christine; Machl, Andy; Zybarth, Gabriele; Richard, Judson; Bockovich, Nick; Kluge, Art; Kley, Nikolai
CORPORATE SOURCE: GPC Biotech, Inc., Waltham, MA, 02451, USA
SOURCE: Chemistry & Biology (Cambridge, MA, United States) (2005), 12(10), 1103-1115
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Cell Press
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 872872-63-4, RGB 310590
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(proteome-wide CDK/CRK-specific kinase inhibitor promotes tumor cell death in absence of cell cycle progression)
RN 872872-63-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(4-methoxyphenyl)methyl]-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)

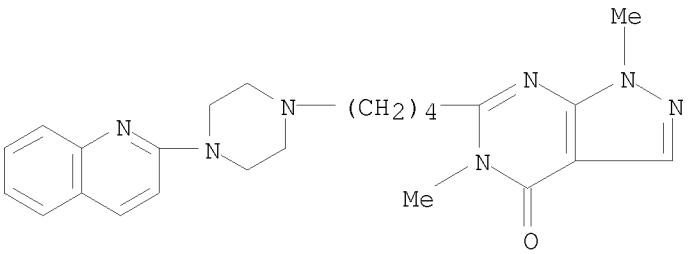


AB The identification of mol. determinants of tumor cell survival is an important objective in cancer research. Here, we describe a small-mol. kinase inhibitor (RGB-286147), which, besides inhibiting tumor cell cycle progression, exhibits potent cytotoxic activity toward noncycling tumor cells, but not nontransformed quiescent fibroblasts. Extensive yeast three-hybrid (Y3H)-based proteome/kinome scanning with chemical dimerizers revealed CDK1/2/3/5/7/9 and the less well-characterized CDK-related kinases (CRKs) p42/CCRK, PCTK1/3, and PFTK1 as its predominant targets. Thus, RGB-286147 is a proteome-wide CDK/CRK-specific kinase inhibitor whose further study could yield new insight into mol. determinants of tumor cell survival. Our results also suggest that the [1,3,6]-tri-substituted-pyrazolo[3,4-d]-pyrimidine-4-one kinase inhibitor scaffold is a promising template for the rational design of kinase inhibitors with potential applications to disease indications other than cancer, such as neurodegeneration, cardiac hypertrophic growth, and AIDS.
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:979639 CAPLUS
DOCUMENT NUMBER: 143:286443
TITLE: Preparation of pyrimidine derivatives as 5-HT3 receptor antagonists having agonistic activity on 5-HT1A
INVENTOR(S): Sato, Michitaka; Matsui, Teruaki; Asagarasu, Akira; Hayashi, Hiroyuki; Araki, Seiichi; Tamaoki, Satoru; Takahashi, Nobuyuki; Yamauchi, Yukinao; Yamamoto, Yoshiko; Yamamoto, Norio; Ogawa, Chisato
PATENT ASSIGNEE(S): Teikoku Hormone Mfg. Co., Ltd., Japan
SOURCE: PCT Int. Appl., 261 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082887	A1	20050909	WO 2005-JP3691	20050225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005217320	A1	20050909	AU 2005-217320	20050225
CA 2557541	A1	20050909	CA 2005-2557541	20050225
EP 1724267	A1	20061122	EP 2005-719969	20050225
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1922171	A	20070228	CN 2005-80005603	20050225
KR 2006127156	A	20061211	KR 2006-717068	20060824
US 20070197551	A1	20070823	US 2006-590707	20060825
PRIORITY APPLN. INFO.:			JP 2004-52040 A	20040226
			JP 2004-322858 A	20041105
			WO 2005-JP3691 W	20050225

OTHER SOURCE(S): MARPAT 143:286443
IT 864386-94-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as 5-HT3 receptor antagonists having agonistic activity on 5-HT1A for treatment of anxiety, depression, etc.)
RN 864386-94-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,5-dimethyl-6-[4-[4-(2-quinolinyl)-1-piperazinyl]butyl]- (CA INDEX NAME)



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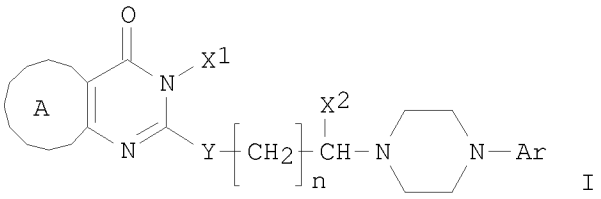

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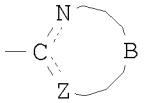


II

AB Title compds. I [ring A = carbocyclic group, etc.; X1 = H, amino, etc.; X2 = H, alkyl; Y = bond, etc.; n = 0-4; Ar = optionally substituted II with halo, etc.; Z = O, etc.; B = moiety required for completing mono-, ploy-heterocyclic ring containing N together with N-C-Z; dotted line indicates single, double bond] were prepared For example, treatment of potassium 3-amino-5,6-dimethyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-2-thiolate with 2-[4-(3-chloropropyl)piperazin-1-yl]quinoline, e.g., prepared from piperazine in 2 steps, afforded 3-amino-5,6-dimethyl-2-[3-(4-quinolin-2-ylpiperazin-1-yl)propylthio]-3H-thieno[2,3-d]pyrimidin-4-one (III) in 50% yield. In 5-HT3 receptor affinity assay (in vitro), compound III exhibited the antagonistic activity of 94% at 10-7 M. Compds. I are claimed useful for the treatment of anxiety, depression, etc. Formulation is given.

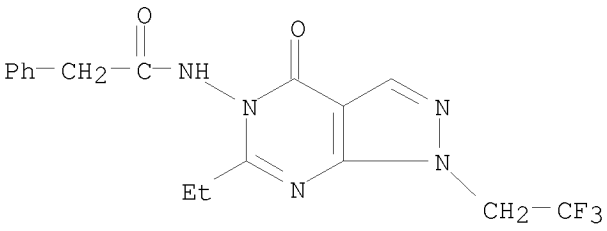
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:238744 CAPLUS
DOCUMENT NUMBER: 142:316851
TITLE: Preparation of fused ring heterocycles as potassium channel modulators
INVENTOR(S): McNaughton-Smith, Grant Andrew; Amato, George Salvatore; Thomas, James Barnwell
PATENT ASSIGNEE(S): Icagen, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 39 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050059823	A1	20050317	US 2004-937958	20040910
US 7223768	B2	20070529		
AU 2004272104	A1	20050324	AU 2004-272104	20040910
CA 2536633	A1	20050324	CA 2004-2536633	20040910
WO 2005025293	A2	20050324	WO 2004-US29868	20040910
WO 2005025293	A3	20050616		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1663237	A2	20060607	EP 2004-788717	20040910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2007505143	T	20070308	JP 2006-526375	20040910
US 20080058319	A1	20080306	US 2007-740831	20070426

PRIORITY APPLN. INFO.:
US 2003-502109P P 20030910
US 2004-937958 A1 20040910
WO 2004-US29868 W 20040910

OTHER SOURCE(S): CASREACT 142:316851; MARPAT 142:316851
IT 848027-62-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinazolines as potassium channel modulators)
RN 848027-62-3 CAPLUS
CN Benzeneacetamide, N-[6-ethyl-1,4-dihydro-4-oxo-1-(2,2,2-trifluoroethyl)-5H-pyrazolo[3,4-d]pyrimidin-5-yl]- (CA INDEX NAME)



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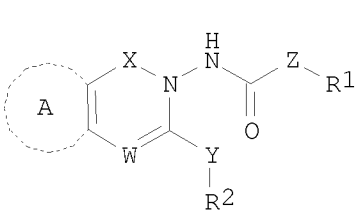

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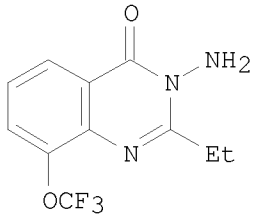


II

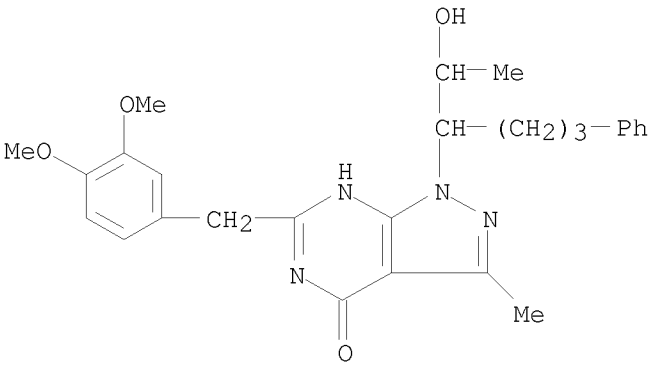
AB Compds. I [A = (un)substituted 5-6 membered (hetero)aryl, cycloalkyl, 5-8 membered heteroaryl; X = CO, CS, SO2; W = N, CR3 (wherein R3 = H, F, (un)substituted (hetero)aryl, etc.); Z = a bond, CH2, CHF, CH:CH, etc.; Y = (CR5R6)n (n = 0-4; R5, R6 = H, F, (un)substituted (hetero)aryl, etc.); R1 = (un)substituted (hetero)aryl, cycloalkyl, 5-7 membered heterocyclyl, alkyl; R2 = CF3, (un)substituted alkyl, (hetero)aryl, cycloalkyl, 3-7 membered heterocyclyl], compns. and methods are provided which are useful in the treatment of diseases through the modulation of potassium ion flux through voltage-dependent potassium channels. More particularly, the invention provides quinazolinones, compns. and methods that are useful in the treatment of central or peripheral nervous system disorders (e.g., migraine, ataxia, Parkinson's disease, bipolar disorders, trigeminal neuralgia, spasticity, mood disorders, brain tumors, psychotic disorders, myokymia, seizures, epilepsy, hearing and vision loss, Alzheimer's disease, age-related memory loss, learning deficiencies, anxiety and motor neuron diseases, maintaining bladder control or treating urinary incontinence) and as neuroprotective agents (e.g., to prevent stroke and the like) by modulating potassium channels associated with the onset or recurrence of the indicated conditions. E.g., a multi-step synthesis of II, starting from 2-trifluoromethoxyaniline, was given. The compound II and analogs were subsequently coupled with isocyanates and carboxylic acids to provide the compds. I such as 1-(2-cyclohexyl-4-oxo-4H-quinazolin-3-yl)-3-(2-fluorobenzyl)urea. The representative compds. I were tested for the ability to open voltage-gated potassium channels in the NG-108-15 FLIPR assay (data given for selected compds. I).

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:216706 CAPLUS
DOCUMENT NUMBER: 142:274026
TITLE: pulmonary surfactant and pde2 inhibitor combinations for treatment of pulmonary diseases
INVENTOR(S): Wollin, Stefan-Lutz
PATENT ASSIGNEE(S): Altana Pharma AG, Germany
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005021037	A1	20050310	WO 2004-EP51948	20040827
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004268387	A1	20050310	AU 2004-268387	20040827
CA 2536458	A1	20050310	CA 2004-2536458	20040827
EP 1660132	A1	20060531	EP 2004-786242	20040827
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2007504117	T	20070301	JP 2006-524370	20040827
US 20060229242	A1	20061012	US 2006-568817	20060221
PRIORITY APPLN. INFO.:			EP 2003-19447 A	20030828
			WO 2004-EP51948 W	20040827

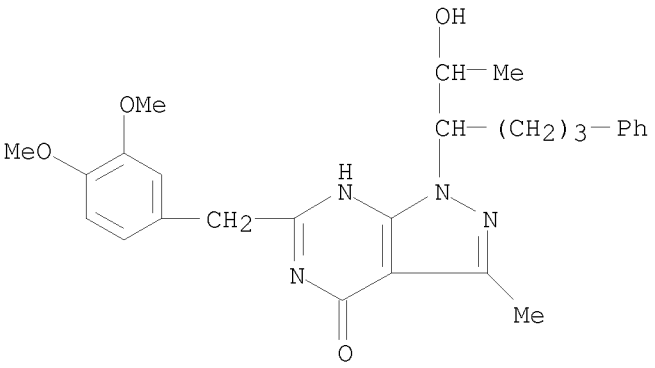
IT 213324-52-8 847472-03-1
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pulmonary surfactant and PDE2 inhibitor combinations for treatment of pulmonary diseases)
RN 213324-52-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]-3-methyl- (CA INDEX NAME)



RN 847472-03-1 CAPLUS
CN 2-35-Lipoprotein SP-C, 5-L-phenylalanine-6-L-phenylalanine-33-L-isoleucine-, mixt. with 6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]-3-methyl-4H-pyrazolo[3,4-d]pyrimidin-4-one (9CI) (CA INDEX NAME)

CM 1

CRN 213324-52-8
CMF C27 H32 N4 O4



CM 2

CRN 200074-80-2
CMF C182 H310 N40 O35
CCI MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

AB The invention relates to the combined administration of a pulmonary surfactant and a PDE2 inhibitor for the treatment of a disease in which pulmonary surfactant malfunction and/or phosphodiesterase 2 (PDE2) activity is detrimental. The invention discloses pharmaceutical compns. comprised of PDE2 inhibitors in combination with pulmonary surfactants for the treatment of lung diseases and injuries.

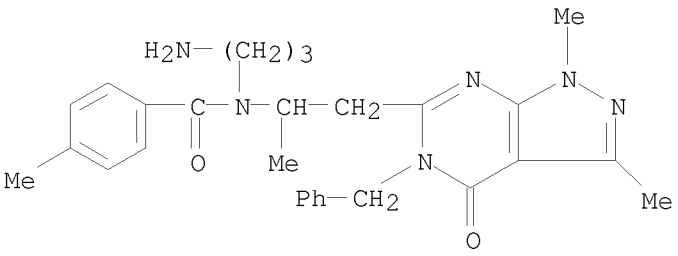
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:1038663 CAPLUS
DOCUMENT NUMBER: 142:6555
TITLE: Preparation of bicyclic pyrimidones as Eg5 modulators for treatment of cancer
INVENTOR(S): Kim, Kyoung S.; Lu, Songfeng; Sheng, X. Christopher; Crews, Alvin Donald
PATENT ASSIGNEE(S): Bristol-Myers Squibb Co., USA
SOURCE: U.S. Pat. Appl. Publ., 39 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040242596	A1	20041202	US 2004-848089	20040518
US 7022850	B2	20060404		
WO 2004106492	A2	20041209	WO 2004-US15972	20040521
WO 2004106492	A3	20050519		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1628981	A2	20060301	EP 2004-752900	20040521
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				

PRIORITY APPLN. INFO.: US 2003-472880P P 20030522
WO 2004-US15972 W 20040521

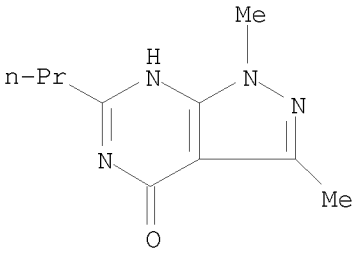
OTHER SOURCE(S): MARPAT 142:6555
IT 799295-87-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(anticancer agent; preparation of bicyclic pyrimidones as Eg5 modulators for treatment of cancer)
RN 799295-87-7 CAPLUS
CN Benzamide, N-(3-aminopropyl)-N-[2-[4,5-dihydro-1,3-dimethyl-4-oxo-5-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-1-methylethyl]-4-methyl-, hydrochloride (1:1) (CA INDEX NAME)



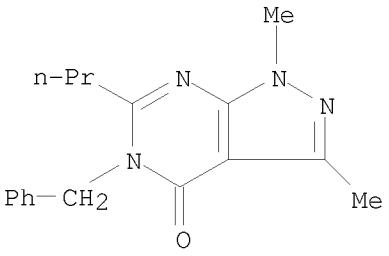
● HCl

IT 799295-88-8P, 1,3-Dimethyl-6-propyl-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one 799295-89-9P, 1,3-Dimethyl-5-benzyl-6-propyl-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one 799295-90-2P, 1,3-Dimethyl-5-benzyl-6-(α-bromopropyl)-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one 799295-91-3P, 1,3-Dimethyl-5-benzyl-6-[2-[[3-[(tert-butoxycarbonyl)amino]propyl]amino]propyl]-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of bicyclic pyrimidones as Eg5 modulators for treatment of cancer)

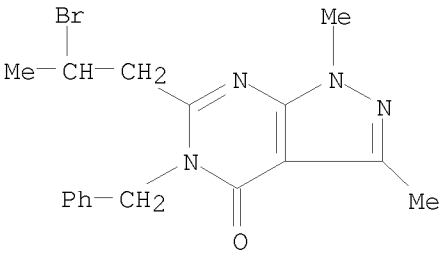
RN 799295-88-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,3-dimethyl-6-propyl- (CA INDEX NAME)



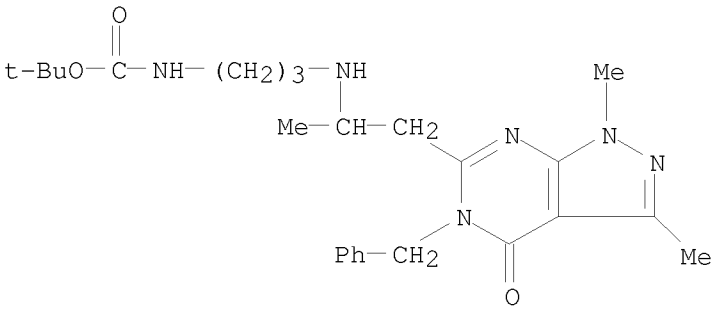
RN 799295-89-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,3-dimethyl-5-(phenylmethyl)-6-propyl- (CA INDEX NAME)



RN 799295-90-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-bromopropyl)-1,5-dihydro-1,3-dimethyl-5-(phenylmethyl)- (CA INDEX NAME)



RN 799295-91-3 CAPLUS
CN Carbamic acid, [3-[[2-[4,5-dihydro-1,3-dimethyl-4-oxo-5-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-6-yl]-1-methylethyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

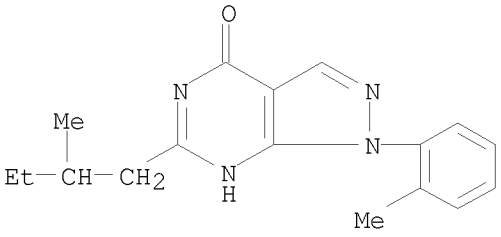
AB Title isoxazolopyrimidinones, pyrazolopyrimidinones, and isothiazolopyrimidinones I or II [wherein X = O, S, N; provided that if X

= O or S, then Y2 is absent; Y1 = H, (un)substituted (cyclo)alkyl, aryl; Y2 = absent, H, alkyl; Z = O, X; R1 = H, (un)substituted alkyl, aryl, (hetero)arylalkyl; R2, R3 = independently H, (cyclo)alkyl, halo; or CR2R3 = cycloalkyl; n = 1, 2; A = N; R4 = COR9, CO2R10, CONR11R12, SO2R13, (un)substituted (cyclo)alkyl, (hetero)aryl; R5, R9-R13 = independently H, (un)substituted (cyclo)alkyl, (hetero)aryl] were prepared as Eg5 modulators (no data). I and II induce mitotic arrest, thereby making them useful as anticancer agents. For example, cycloaddn. of 2-(1-ethoxyethylidene)malononitrile and hydroxylamine•HCl gave 5-amino-3-methylisoxazole-4-carbonitrile (72%), which was coupled with butyric anhydride to provide 3-methyl-6-propyl-5H-isoxazolo[5,4-d]pyrimidin-4-one (52%). The isoxazol[5,4-d]pyrimidin-4-one was then benzylated (20%), brominated (30%), aminated with 1,3-diaminopropane (66%), acylated with 4-toluoyl chloride (95%), and deprotected (65%) to afford III. Compds. of the invention exhibited activity in a 72-h cell proliferation assay, inhibiting cell proliferation against one or more of ovarian, breast, prostate, lung, leukemia, or colorectal human cancer cell lines with IC50 values ≤10 μM. I and II also exhibited activity in a clonogenecity assay and a cell cycle profile anal. assay, producing significant increases in mitotic and apoptotic fractions of the cell population. Addnl., invention compds. inhibited bipolar spindle formation and induced a monoastral array of microtubules in immunocytochem. assays. Thus, I, II, and their pharmaceutical compns., optionally in combination with at least one other anticancer agent, are useful for the treatment of cancer and other proliferative disorders.

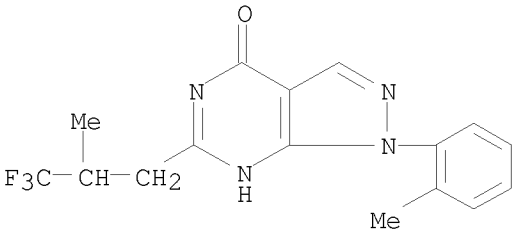
L4 ANSWER 15 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:996183 CAPLUS
DOCUMENT NUMBER: 141:424206
TITLE: Preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics.
INVENTOR(S): Hendrix, Martin; Baerfacker, Lars; Erb, Christina; Hafner, Frank-Thorsten; Heckroth, Heike; Schauss, Dagmar; Tersteegen, Adrian; Van Der Staay, Franz-Josef; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099211	A1	20041118	WO 2004-EP4455	20040428
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004004142	A1	20041125	DE 2004-102004004142	20040128
AU 2004235915	A1	20041118	AU 2004-235915	20040428
CA 2524900	A1	20041118	CA 2004-2524900	20040428
EP 1626971	A1	20060222	EP 2004-729876	20040428
R: DE, ES, FR, GB, IT				
JP 2006525966	T	20061116	JP 2006-505294	20040428
US 20070105876	A1	20070510	US 2005-556224	20051109
IN 2005DN05418	A	20070928	IN 2005-DN5418	20051124
PRIORITY APPLN. INFO.:			DE 2003-10320784 A	20030509
			DE 2003-10336183 A	20030807
			DE 2004-102004004142A	20040128
			WO 2004-EP4455 W	20040428

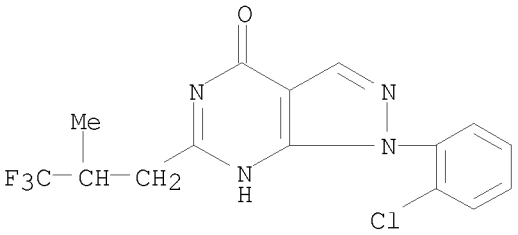
OTHER SOURCE(S): MARPAT 141:424206
IT 794568-84-6P 794568-87-9P 794568-90-4P
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)
RN 794568-84-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(2-methylbutyl)-1-(2-methylphenyl)- (CA INDEX NAME)



RN 794568-87-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylphenyl)-6-(3,3,3-trifluoro-2-methylpropyl)- (CA INDEX NAME)

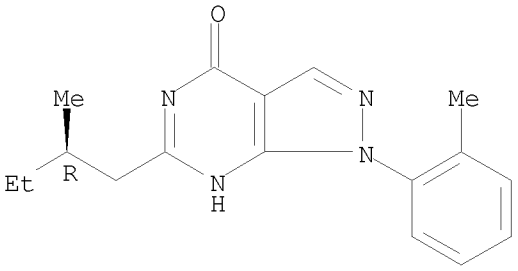


RN 794568-90-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-1,5-dihydro-6-(3,3,3-trifluoro-2-methylpropyl)- (CA INDEX NAME)



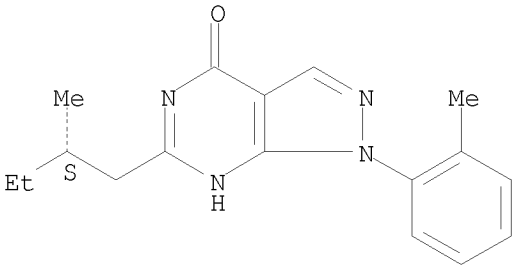
IT 794568-85-7P 794568-86-8P 794568-88-0P
794568-89-1P 794568-91-5P 794568-92-6P
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)
RN 794568-85-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2R)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.



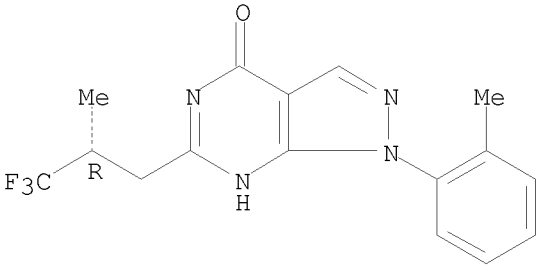
RN 794568-86-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[(2S)-2-methylbutyl]-1-(2-methylphenyl)- (CA INDEX NAME)

Absolute stereochemistry.



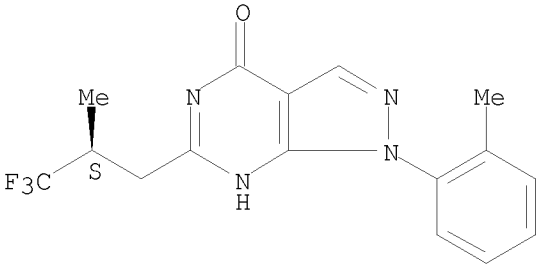
RN 794568-88-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.



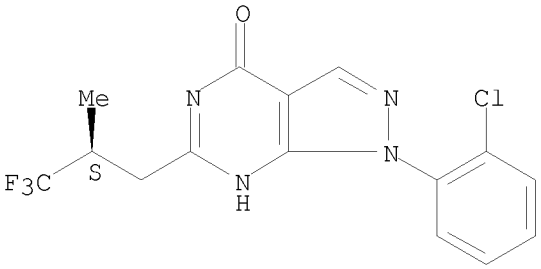
RN 794568-89-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylphenyl)-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.



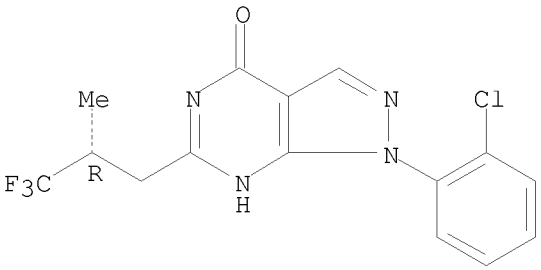
RN 794568-91-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-chlorophenyl)-1,5-dihydro-6-[(2S)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.



RN 794568-92-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-chlorophenyl)-1,5-dihydro-6-[(2R)-3,3,3-trifluoro-2-methylpropyl]-
(CA INDEX NAME)

Absolute stereochemistry.



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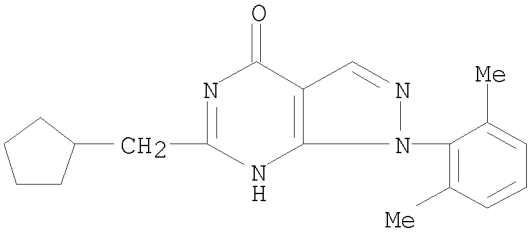
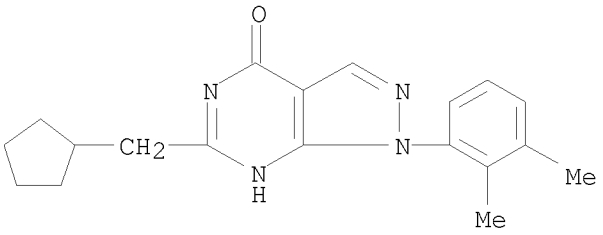
794568-59-5P 794568-60-8P 794568-61-9P
794568-62-0P 794568-63-1P 794568-64-2P
794568-65-3P 794568-67-5P 794568-68-6P
794568-69-7P 794568-70-0P 794568-71-1P

794568-72-2P 794568-73-3P 794568-74-4P
794568-75-5P 794568-76-6P 794568-79-9P
794568-80-2P 794568-81-3P 794568-82-4P
794568-83-5P 794568-97-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as phosphodiesterase 9A inhibitors useful as nootropics)

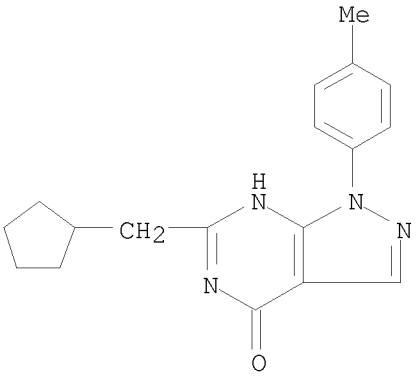
RN 794568-50-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,6-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



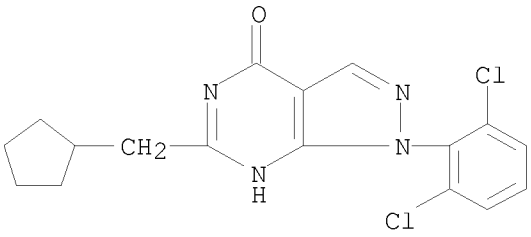
RN 794568-51-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,3-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



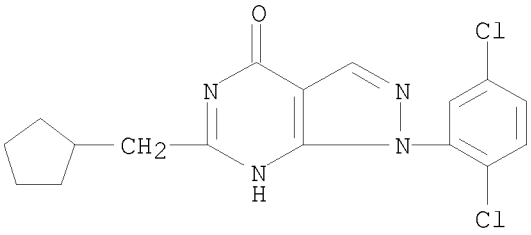
RN 794568-52-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methylphenyl)- (CA INDEX NAME)



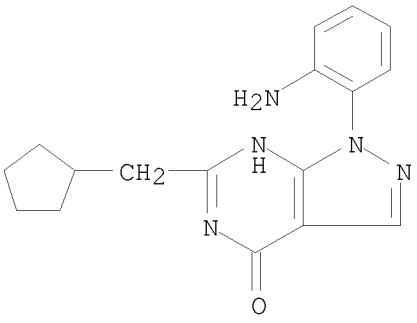
RN 794568-53-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2,6-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



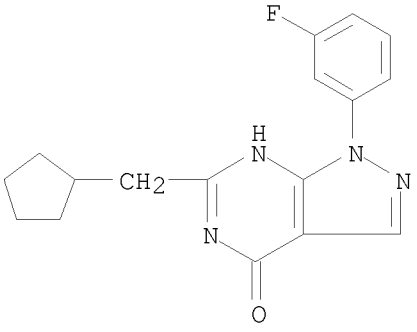
RN 794568-54-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2,5-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



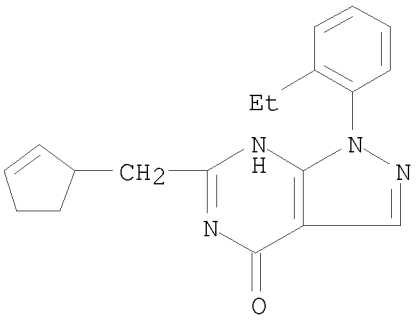
RN 794568-55-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(2-aminophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)



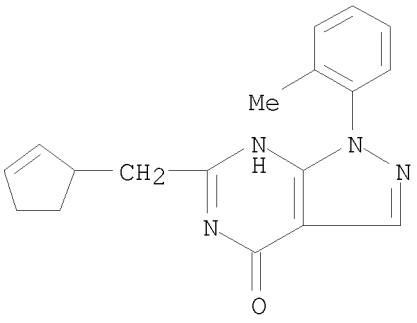
RN 794568-56-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(3-fluorophenyl)-1,5-dihydro- (CA INDEX NAME)



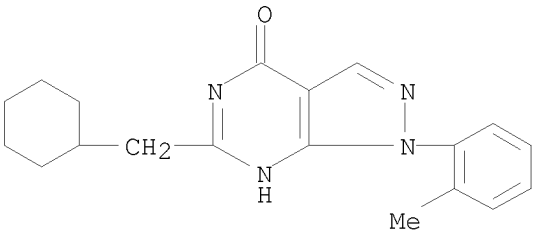
RN 794568-57-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-(2-ethylphenyl)-1,5-dihydro- (CA INDEX NAME)



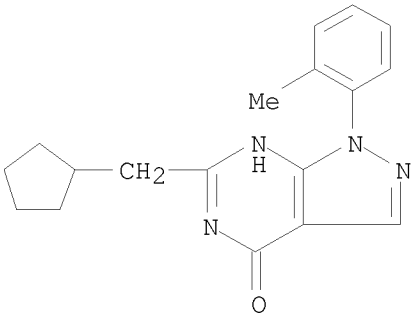
RN 794568-58-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



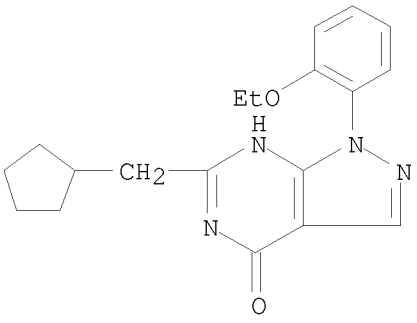
RN 794568-59-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclohexylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



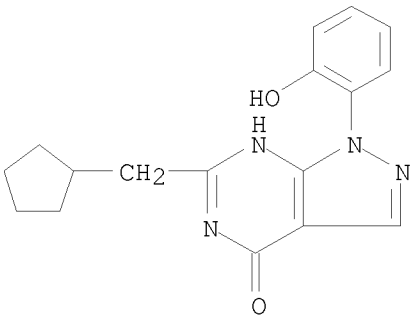
RN 794568-60-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



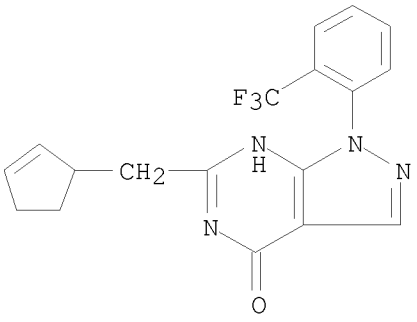
RN 794568-61-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(2-ethoxyphenyl)-1,5-dihydro- (CA INDEX NAME)



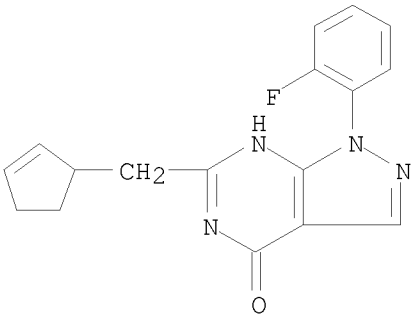
RN 794568-62-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(2-hydroxyphenyl)- (CA INDEX NAME)



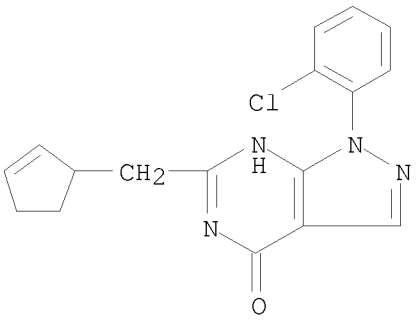
RN 794568-63-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-[2-(trifluoromethyl)phenyl]-
(CA INDEX NAME)



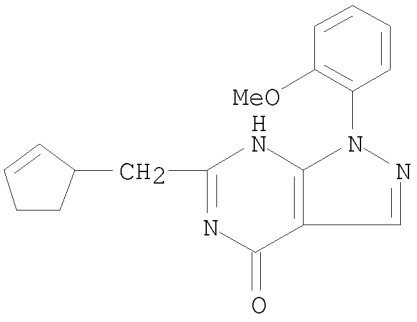
RN 794568-64-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(2-cyclopenten-1-ylmethyl)-1-(2-fluorophenyl)-1,5-dihydro- (CA INDEX
NAME)



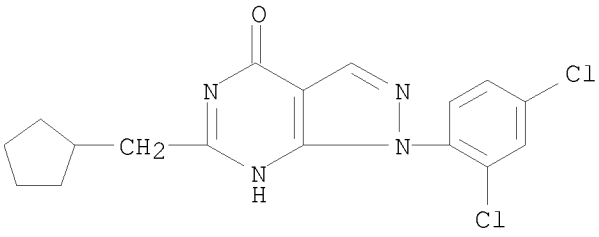
RN 794568-65-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chlorophenyl)-6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro- (CA INDEX NAME)



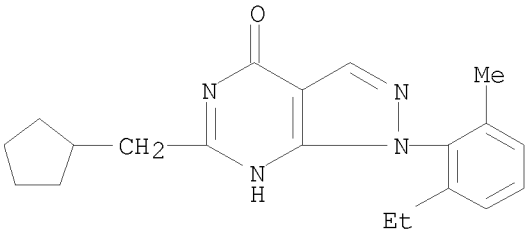
RN 794568-67-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1,5-dihydro-1-(2-methoxyphenyl)- (CA INDEX NAME)



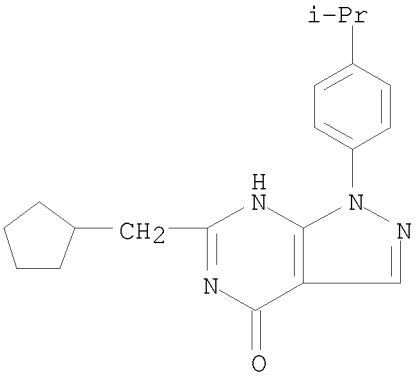
RN 794568-68-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



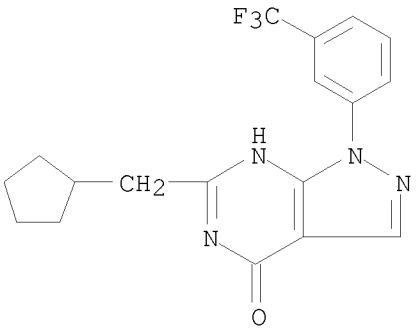
RN 794568-69-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1-(2-ethyl-6-methylphenyl)-1,5-dihydro- (CA INDEX NAME)



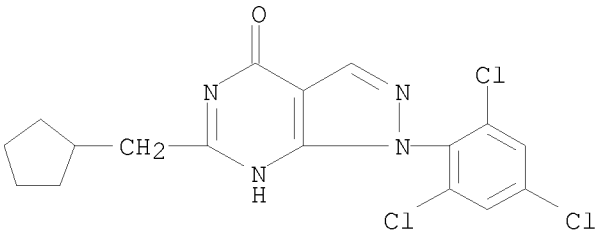
RN 794568-70-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



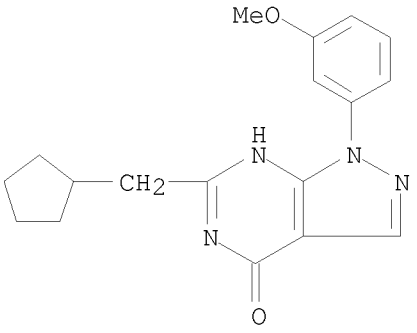
RN 794568-71-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclopentylmethyl)-1,5-dihydro-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



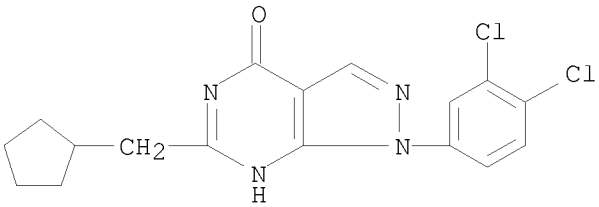
RN 794568-72-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(2,4,6-trichlorophenyl)- (CA INDEX NAME)



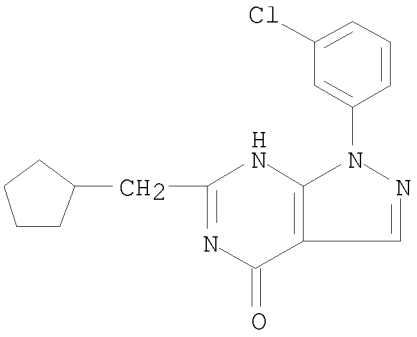
RN 794568-73-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1,5-dihydro-1-(3-methoxyphenyl)- (CA INDEX NAME)



RN 794568-74-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(3,4-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



RN 794568-75-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(3-chlorophenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)



RN 794568-76-6 CAPLUS
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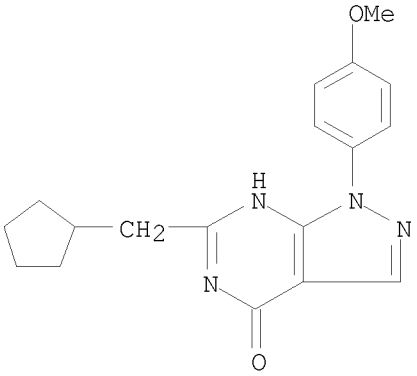
6-(cyclopentylmethyl)-1,5-dihydro-1-(4-methoxyphenyl)- (CA INDEX NAME)



RN 794568-79-9 CAPLUS
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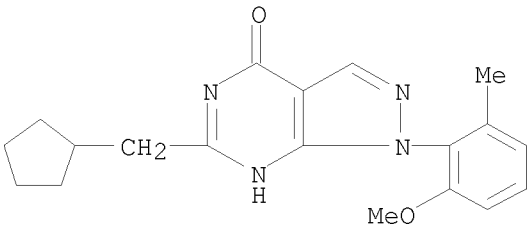
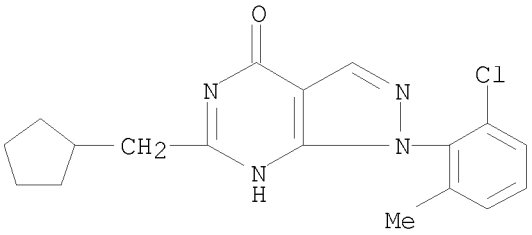
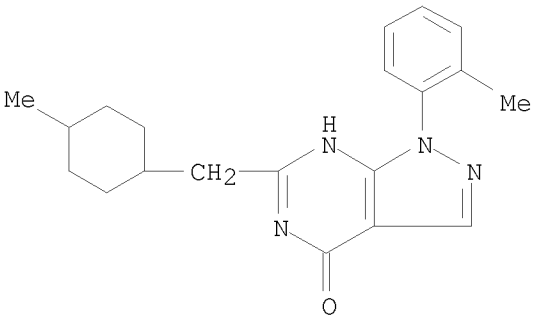
6-(cyclopentylmethyl)-1,5-dihydro-1-(2-methoxy-6-methylphenyl)- (CA INDEX NAME)



RN 794568-80-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(2-chloro-6-methylphenyl)-6-(cyclopentylmethyl)-1,5-dihydro- (CA INDEX NAME)

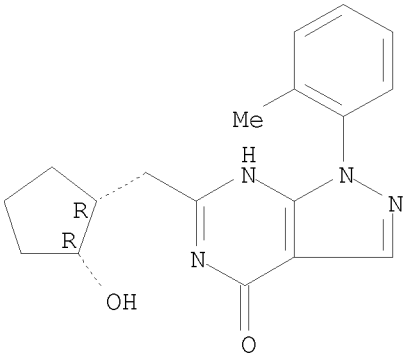


RN 794568-81-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(4-methylcyclohexyl)methyl]-1-(2-methylphenyl)- (CA INDEX NAME)



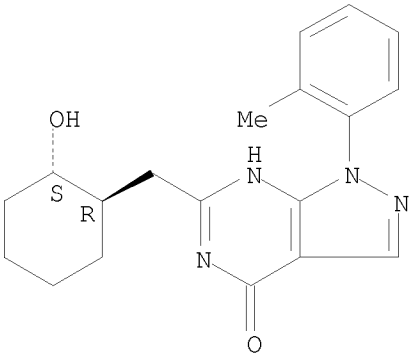
RN 794568-82-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[[(1R,2R)-2-hydroxycyclopentyl]methyl]-1-(2-methylphenyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 794568-83-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[[(1R,2S)-2-hydroxycyclohexyl]methyl]-1-(2-methylphenyl)-,
rel- (CA INDEX NAME)

Relative stereochemistry.



RN 794568-97-1 CAPLUS
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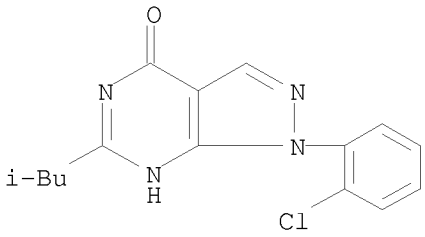
1-(2-chlorophenyl)-1,5-dihydro-6-(2-methylpropyl)- (CA INDEX NAME)



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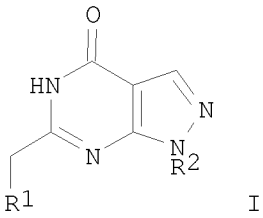

I

AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = (substituted) Ph, heteroaryl], were prepared Thus, reflux of 5-amino-1-(2-methylphenyl)-1H-pyrazole-4-carboxamide (preparation given) with Et cyclopentylacetate and NaH in EtOH overnight gave 30% 6-cyclopentylmethyl-1-(2-methylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one. The latter inhibited PDE9A with IC50 = 5 nM.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:996182 CAPLUS
DOCUMENT NUMBER: 141:410967
TITLE: Preparation of 6-arylmethylpyrazolopyrimidines as PDE9A inhibitors for the treatment of Alzheimer's disease
INVENTOR(S): Hendrix, Martin; Baerfacker, Lars; Erb, Christina; Hafner, Frank-Thorsten; Heckroth, Heike; Schauss, Dagmar; Tersteegen, Adrian; Van Der Staay, Franz-Josef; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004099210	A1	20041118	WO 2004-EP4412	20040427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10320785	A1	20041125	DE 2003-10320785	20030509
CA 2524898	A1	20041118	CA 2004-2524898	20040427
EP 1628980	A1	20060301	EP 2004-739107	20040427
R: DE, ES, FR, GB, IT				
JP 2006525963	T	20061116	JP 2006-505276	20040427
US 20070161662	A1	20070712	US 2006-556437	20061010

PRIORITY APPLN. INFO.: DE 2003-10320785 A 20030509
WO 2004-EP4412 W 20040427

IT 792952-76-2P, 6-(3-Chlorobenzyl)-1-(2,6-dimethylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-77-3P, 6-(3-Chlorobenzyl)-1-(2,3-dimethylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-78-4P, 6-(3-Chlorobenzyl)-1-(4-methylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-79-5P, 6-(3-Chlorobenzyl)-1-(2,6-dichlorophenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-80-8P, 6-(3-Chlorobenzyl)-1-(2,5-dichlorophenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-81-9P, 1-(2-Aminophenyl)-6-(3-chlorobenzyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-82-0P, 6-(3-Chlorobenzyl)-1-(3-fluorophenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-84-2P, 6-(2-Bromobenzyl)-1-(2-methylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-85-3P, 6-(3-Bromobenzyl)-1-(2-methylphenyl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one 792952-86-4P 792952-87-5P 792952-88-6P 792952-89-7P 792952-90-0P 792952-91-1P,

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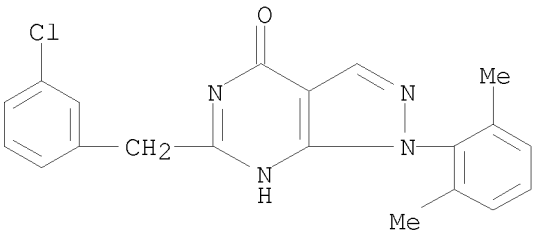
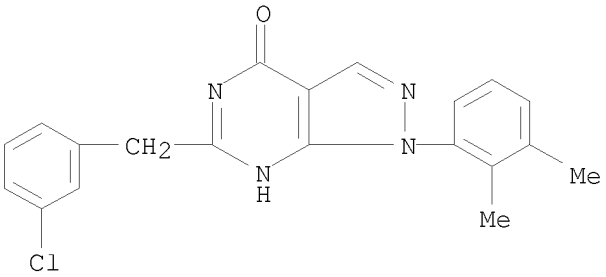
6-(3-Chlorobenzyl)-1-(2-trifluoromethylphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-95-5P,
6-(3-Chlorobenzyl)-1-(2-fluorophenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-96-6P,
6-(3-Chlorobenzyl)-1-(2-chlorophenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one 792952-98-8P,
6-(3-Chlorobenzyl)-1-(2-methoxyphenyl)-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylmethylpyrazolopyrimidines as PDE9A inhibitors for the treatment of Alzheimer's disease)

RN 792952-76-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(2,6-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



RN 792952-77-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(2,3-dimethylphenyl)-1,5-dihydro- (CA INDEX NAME)



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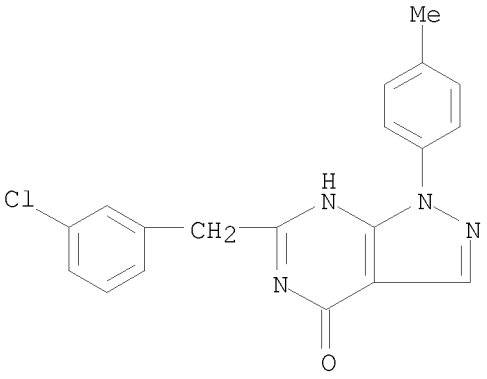

RN 792952-79-5 CAPLUS
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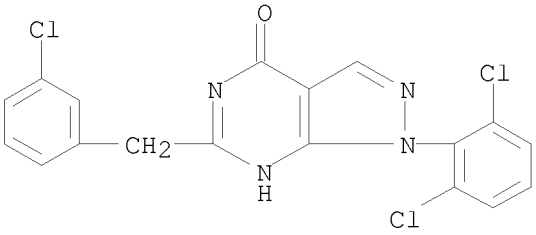
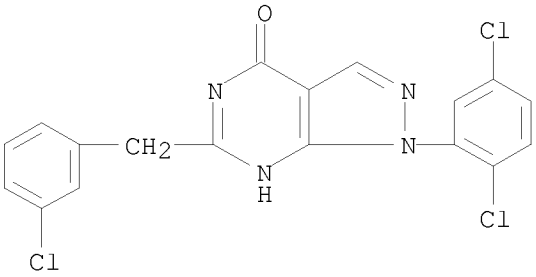


RN 792952-80-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-(2,5-dichlorophenyl)-1,5-dihydro- (CA INDEX NAME)



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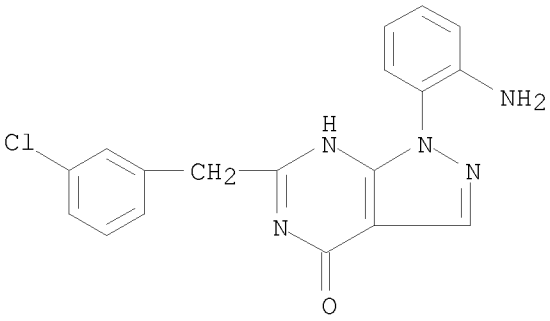

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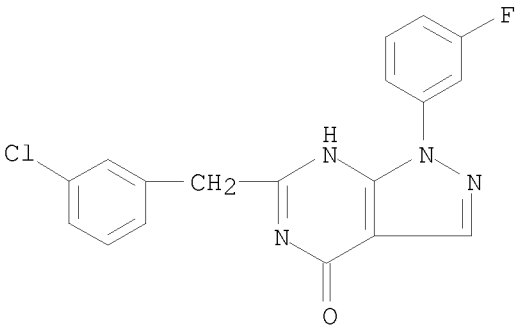

RN 792952-84-2 CAPLUS
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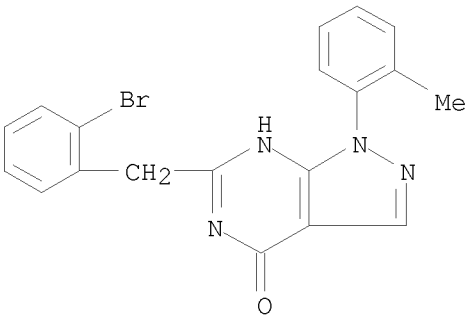

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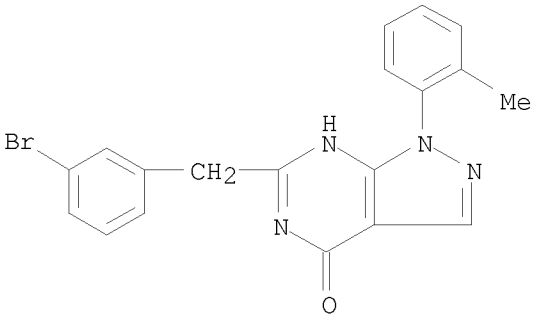

RN 792952-86-4 CAPLUS
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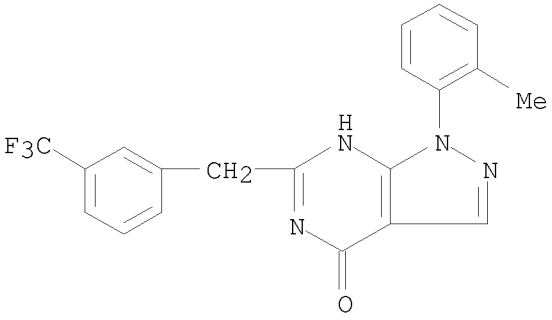

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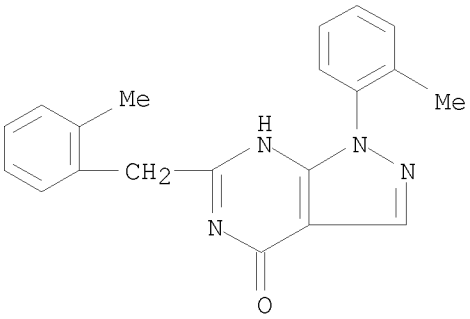

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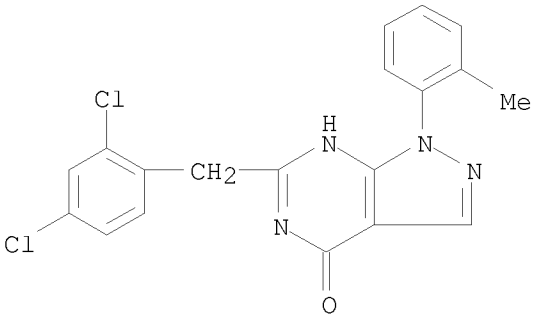

RN 792952-89-7 CAPLUS
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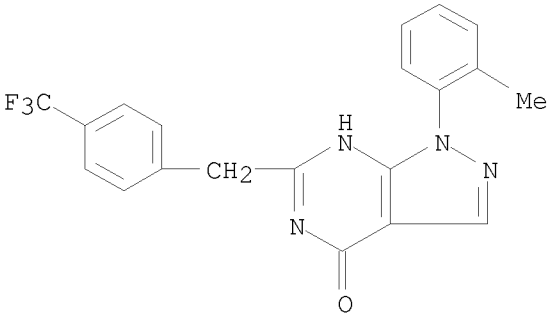

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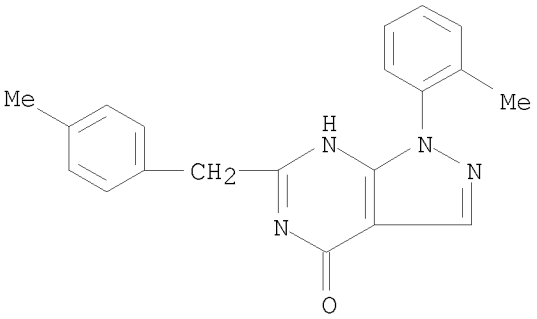
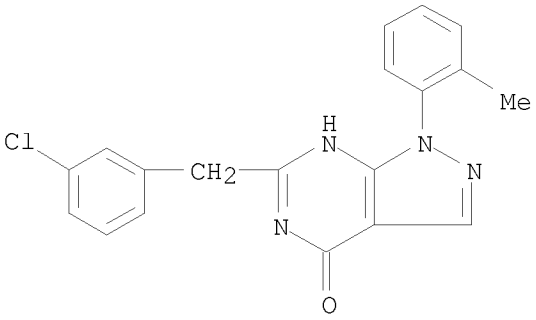


RN 792952-91-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1,5-dihydro-1-(2-methylphenyl)- (CA INDEX NAME)



RN 792952-92-2 CAPLUS
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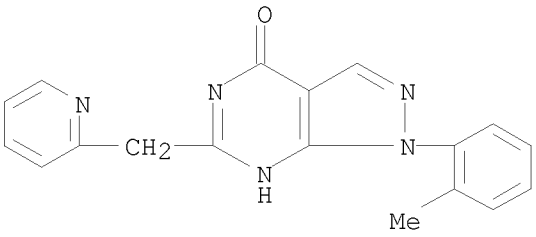

RN 792952-93-3 CAPLUS
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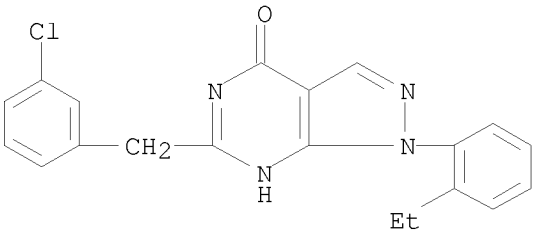
6-[(3-chlorophenyl)methyl]-1-(2-ethylphenyl)-1,5-dihydro- (CA INDEX NAME)



RN 792952-94-4 CAPLUS
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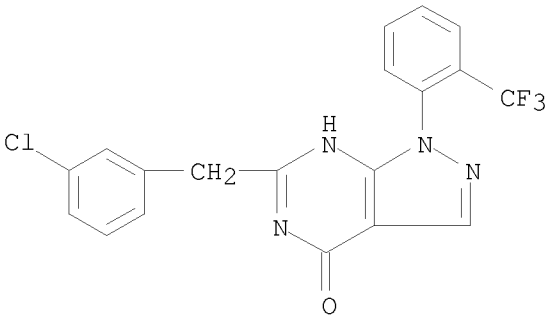

RN 792952-95-5 CAPLUS
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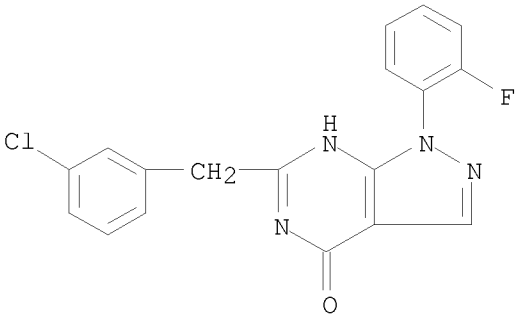

RN 792952-96-6 CAPLUS
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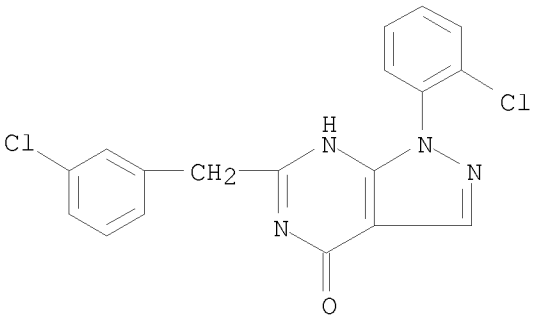
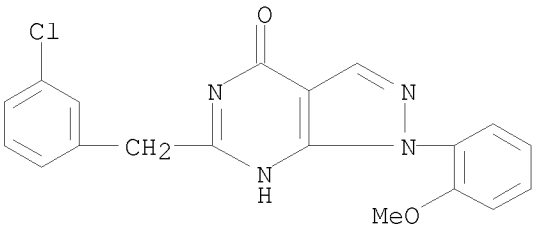
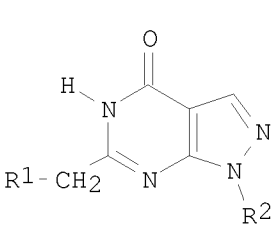


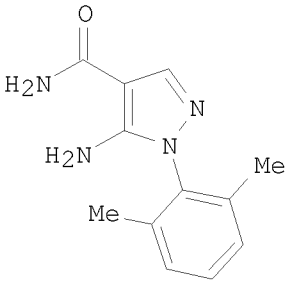
RN 792952-98-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1,5-dihydro-1-(2-methoxyphenyl)- (CA INDEX NAME)



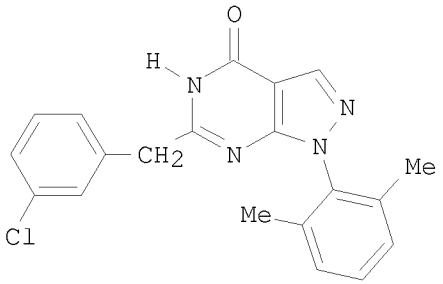
GI



I



II



III

AB Title compds. I [R1 = (un)substituted Ph, pyridyl, thiophenyl, etc.; (un)substituted Ph, heteroaryl] and their pharmaceutically acceptable salts were prepared For example, condensation-cyclization of 3-chlorophenylacetic acid Me ester and aminopyrazole II, e.g., prepared from 2,3-dimethylphenylhydrazine hydrochloride and (ethoxymethylene)propanedinitrile, afforded pyrazolopyrimidine III in 37% yield. In human guanosine cyclic 3,5'-phosphate phosphodiesterase (PDE9A) inhibition assays, 4-examples of compds. I exhibited IC50 values ranging from <30-64 nM. Compds. I are claimed useful for the treatment of Alzheimer's disease.

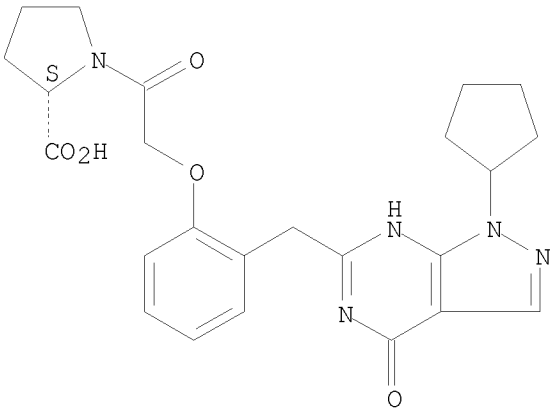
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:934326 CAPLUS
DOCUMENT NUMBER: 141:395571
TITLE: Preparation of pyrazolopyrimidinones as phosphodiesterase 9 (PDE9) inhibitors for treating type 2 diabetes, metabolic syndrome, and cardiovascular disease.
INVENTOR(S): Bell, Andrew Simon; Deninno, Michael Paul; Palmer, Michael John; Visser, Michael Scott
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 26 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

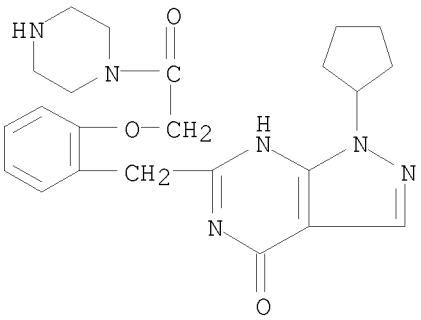
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20040220186	A1	20041104	US 2004-828485	20040420
WO 2004096811	A1	20041111	WO 2004-IB1796	20040421
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
NL 1026091	A1	20041102	NL 2004-1026091	20040429
NL 1026091	C2	20050526		

PRIORITY APPLN. INFO.: US 2003-466639P P 20030430
US 2004-828485 A 20040420
OTHER SOURCE(S): MARPAT 141:395571
IT 787618-74-0P 787618-76-2P 787618-84-2P
787618-85-3P 787618-86-4P 787618-87-5P
787618-88-6P 787618-89-7P 787618-90-0P
787618-92-2P 787618-97-7P 787619-14-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of pyrazolopyrimidinones as PDE9 inhibitors for
treating type 2 diabetes, metabolic syndrome, and cardiovascular disease)
RN 787618-74-0 CAPLUS
CN L-Proline, 1-[[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

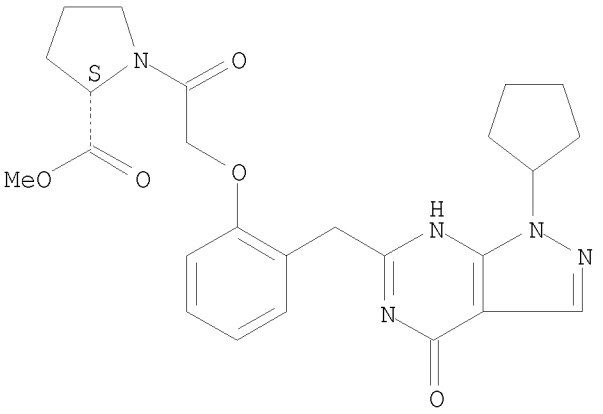


RN 787618-76-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-oxo-2-(1-piperazinyl)ethoxy]phenyl]methyl]- (CA INDEX NAME)

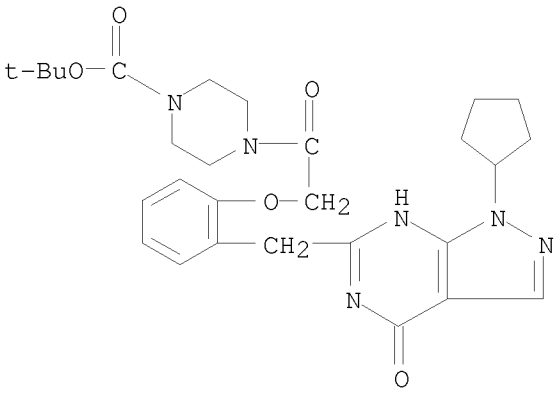


RN 787618-84-2 CAPLUS
CN L-Proline, 1-[[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

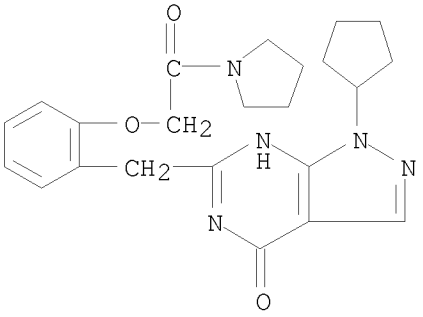
Absolute stereochemistry.



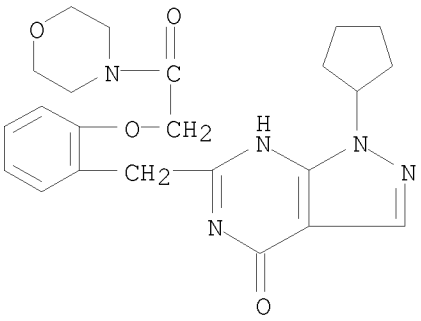
RN 787618-85-3 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]acetyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



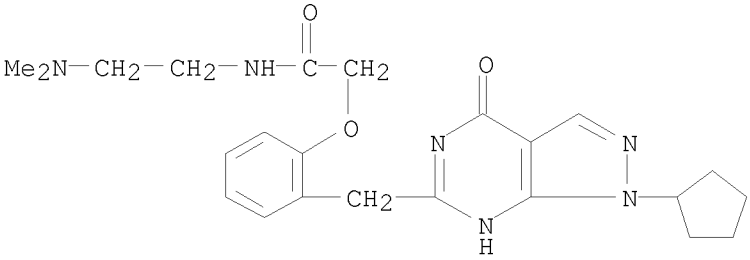
RN 787618-86-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-oxo-2-(1-pyrrolidinyl)ethoxy]phenyl]methyl]- (CA INDEX NAME)



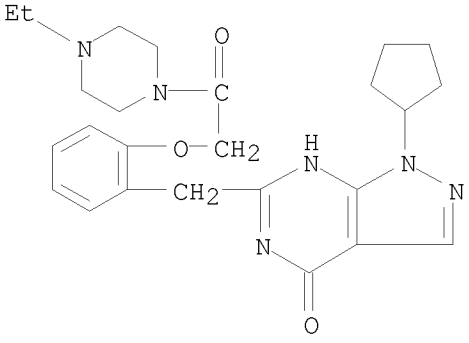
RN 787618-87-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-(4-morpholinyl)-2-oxoethoxy]phenyl]methyl]- (CA INDEX NAME)



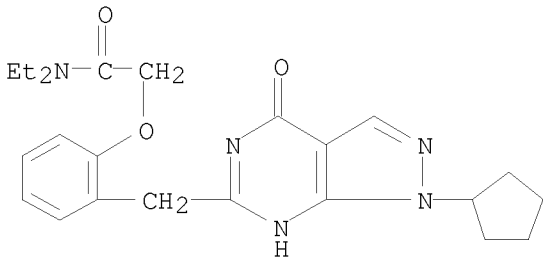
RN 787618-88-6 CAPLUS
CN Acetamide, 2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]-N-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



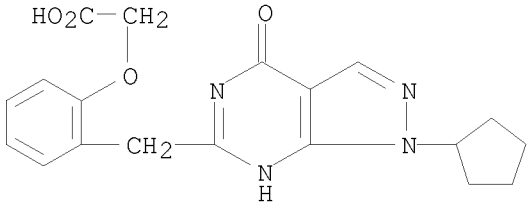
RN 787618-89-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[[2-[2-(4-ethyl-1-piperazinyl)-2-oxoethoxy]phenyl]methyl]-1,5-dihydro- (CA INDEX NAME)



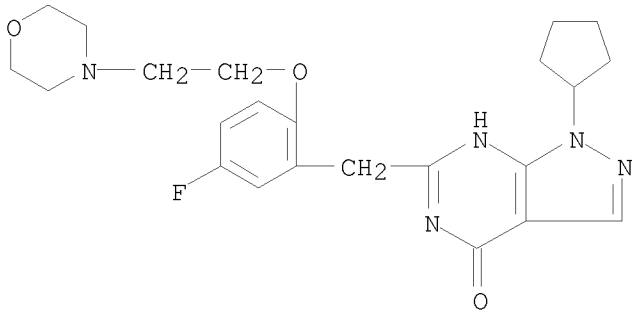
RN 787618-90-0 CAPLUS
CN Acetamide, 2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]-N,N-diethyl- (CA INDEX NAME)



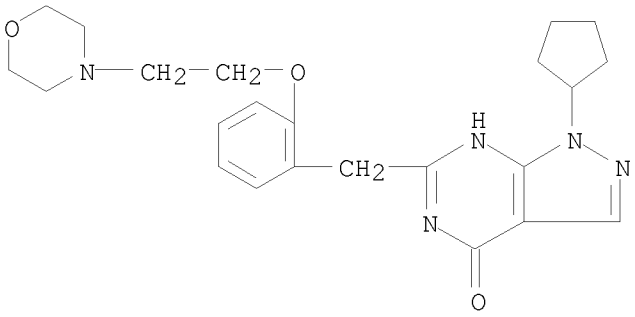
RN 787618-92-2 CAPLUS
CN Acetic acid, 2-[2-[(1-cyclopentyl-4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl)methyl]phenoxy]- (CA INDEX NAME)



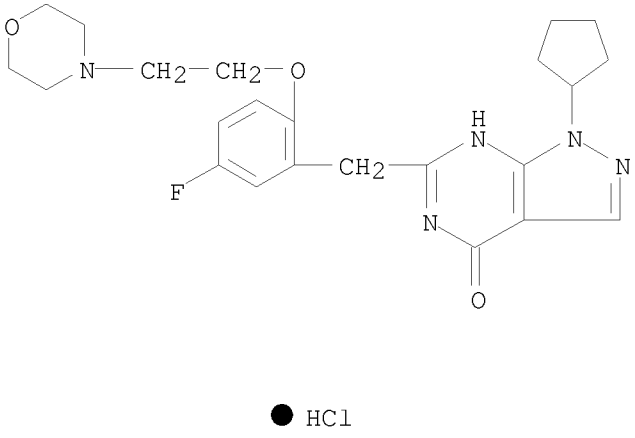
RN 787618-97-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[[5-fluoro-2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]-1,5-dihydro- (CA INDEX NAME)



RN 787619-14-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]- (CA INDEX NAME)

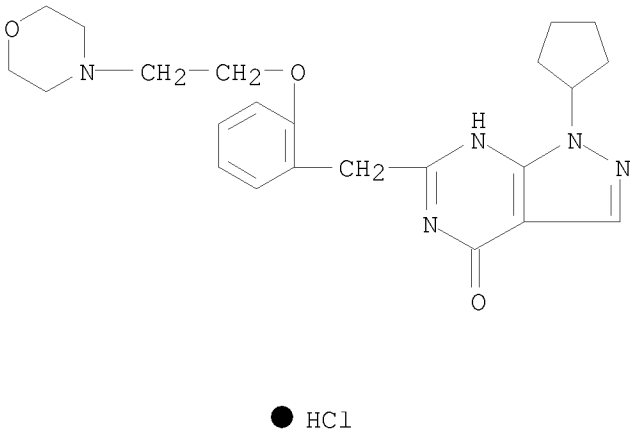


IT 787619-25-4P 787619-37-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as PDE9 inhibitors for treating type 2 diabetes, metabolic syndrome, and cardiovascular disease)
RN 787619-25-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-6-[[5-fluoro-2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]-1,5-dihydro-, hydrochloride (1:1) (CA INDEX NAME)



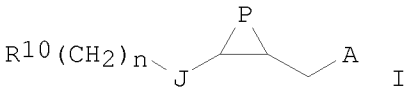
● HCl

RN 787619-37-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[[2-[2-(4-morpholinyl)ethoxy]phenyl]methyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

GI



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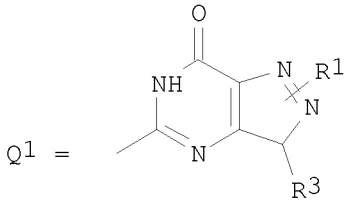
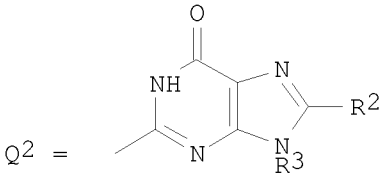


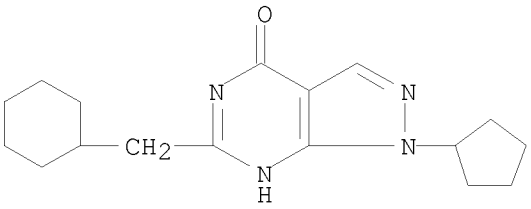


AB Title compds. [I; A = Q1, Q2, etc.; P = atoms to form (substituted) cycloalkyl, heterocycloalkyl, aryl, heteroaryl rings; J = O, S, NR15, NR15CO, NR15SO2; R10 = CO2H, CONR30R31, NR15SO2R40; R1, R2, R15 = H, alkyl; R3 = alkyl, cycloalkyl, cycloalkylmethyl, heterocycloalkyl, heterocycloalkylmethyl, aryl, heteroaryl; R30, R31 = H, (substituted) alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl; R30R31N = (substituted) 5-8 membered heterocyclyl; R40 = H, alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl; n = 1-3], were prepared Thus, Et 1-[[2-(3-isopropyl-7-oxo-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-ylmethyl)phenoxy]acetyl]pyrrolidine-2-carboxylate was heated with aqueous NaOH in MeOH for 2 h at 58° to give after acidification with HCl 1-[[2-(3-isopropyl-7-oxo-6,7-dihydro-1H-pyrazolo[4,3-d]pyrimidin-5-ylmethyl)phenoxy]acetyl]pyrrolidine-2-carboxylic acid. Some compds. inhibited PDE9 with IC50 <50 nM.

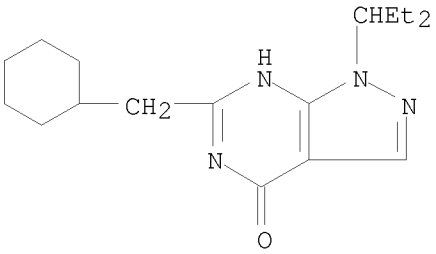
L4 ANSWER 18 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:198173 CAPLUS
DOCUMENT NUMBER: 140:247085
TITLE: Selective phosphodiesterase 9A inhibitors for the improvement of cognitive processes
INVENTOR(S): Boss, Frank-Gerhard; Erb, Christina; Hendrix, Martin; Van Kampen, Marja; Wunder, Frank
PATENT ASSIGNEE(S): Bayer AG, Germany
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238722	A1	20040311	DE 2002-10238722	20020823
CA 2496292	A1	20040401	CA 2003-2496292	20030811
WO 2004026286	A2	20040401	WO 2003-EP8880	20030811
WO 2004026286	A3	20040603		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003258597	A1	20040408	AU 2003-258597	20030811
EP 1534285	A2	20050601	EP 2003-797233	20030811
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006501272	T	20060112	JP 2004-536933	20030811
US 20060100222	A1	20060511	US 2005-525119	20051014
PRIORITY APPLN. INFO.:			DE 2002-10238722 A	20020823
			WO 2003-EP8880 W	20030811

IT 667400-78-4P 667400-79-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phosphodiesterase 9A inhibitors for improvement of cognitive processes)
RN 667400-78-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



RN 667400-79-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclohexylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)

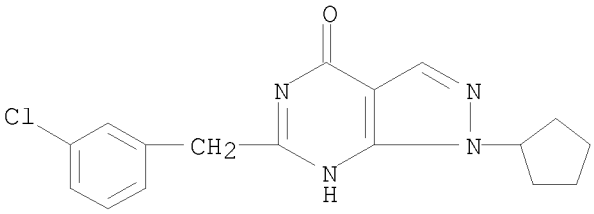


AB The invention discloses the use of selective phosphodiesterase 9A inhibitors for the production of drugs for the improvement of perception, concentration, cognitive processes, learning and/or memory. Preparation and activity of pyrazolopyrimidinone derivs. is included.

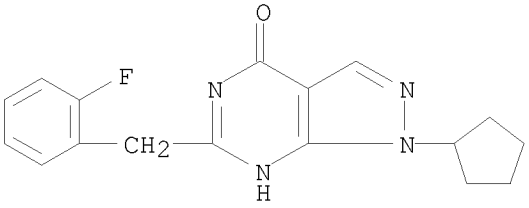
L4 ANSWER 19 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:182883 CAPLUS
DOCUMENT NUMBER: 140:217660
TITLE: Preparation of 6-benzylpyrazolo[3,4-d]pyrimidin-4-ones as phosphodiesterase-9A (PDE9A) inhibitors.
INVENTOR(S): Hendrix, Martin; Boess, Frank-Gerhard; Burkhardt, Nils; Erb, Christina; Tersteegen, Adrian; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018474	A1	20040304	WO 2003-EP8923	20030812
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10238723	A1	20040311	DE 2002-10238723	20020823
CA 2496194	A1	20040304	CA 2003-2496194	20030812
AU 2003258601	A1	20040311	AU 2003-258601	20030812
EP 1534711	A1	20050601	EP 2003-792301	20030812
EP 1534711	B1	20060419		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006507242	T	20060302	JP 2004-530129	20030812
ES 2263057	T3	20061201	ES 2003-792301	20030812
US 20060106035	A1	20060518	US 2005-525115	20050831
PRIORITY APPLN. INFO.:			DE 2002-10238723 A	20020823
			WO 2003-EP8923 W	20030812

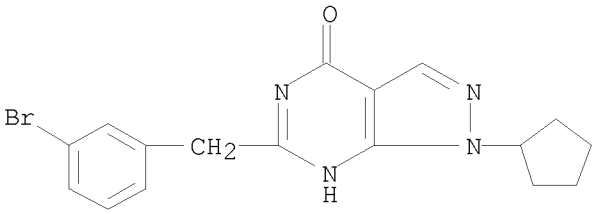
OTHER SOURCE(S): MARPAT 140:217660
IT 666235-19-4P 666235-20-7P 666235-21-8P
666235-22-9P 666235-23-0P 666235-24-1P
666235-25-2P 666235-26-3P 666235-27-4P
666235-28-5P 666235-29-6P 666235-30-9P
666235-31-0P 666235-32-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzylpyrazolopyrimidones as phosphodiesterase-9A (PDE9A) inhibitors)
RN 666235-19-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chlorophenyl)methyl]-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



RN 666235-20-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-cyclopentyl-6-[(2-fluorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



RN 666235-21-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3-bromophenyl)methyl]-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



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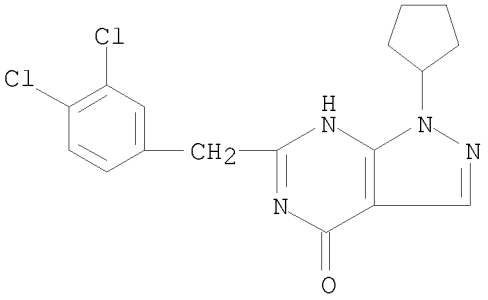
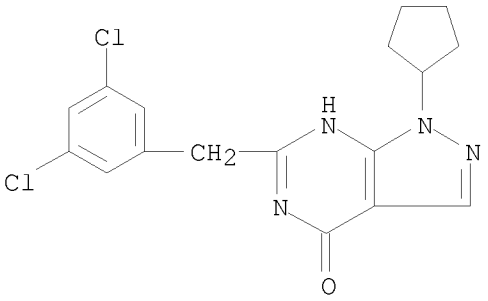


RN 666235-23-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-cyclopentyl-6-[(3,5-dichlorophenyl)methyl]-1,5-dihydro- (CA INDEX NAME)



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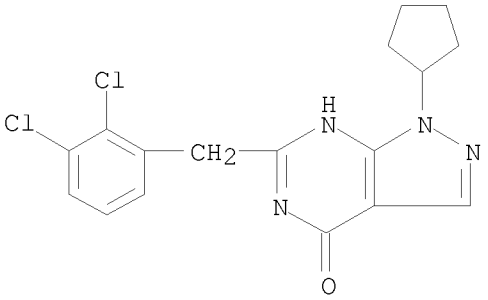

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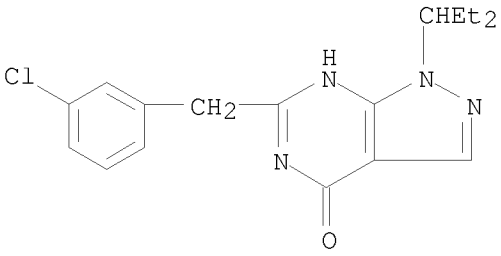

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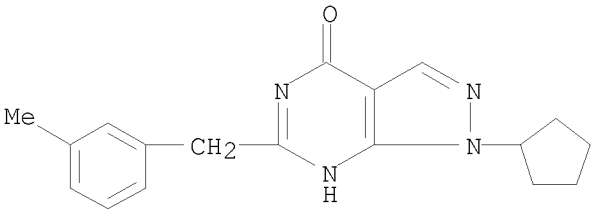

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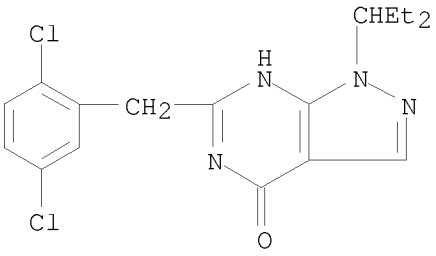

RN 666235-28-5 CAPLUS
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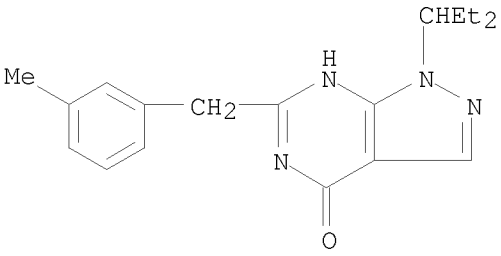
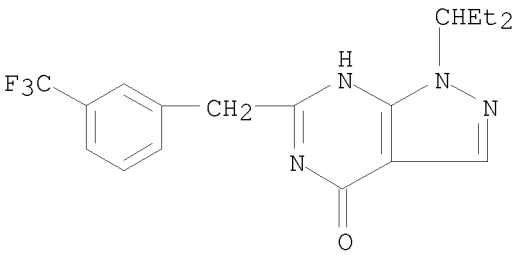
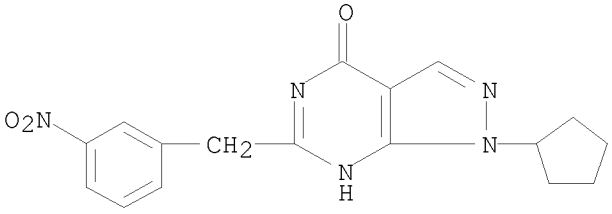


RN 666235-29-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-[[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)



RN 666235-30-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-cyclopentyl-1,5-dihydro-6-[(3-nitrophenyl)methyl]- (CA INDEX NAME)



RN 666235-31-0 CAPLUS
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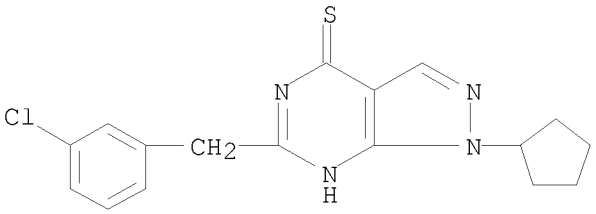
6-[(3-chlorophenyl)methyl]-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



RN 666235-32-1 CAPLUS
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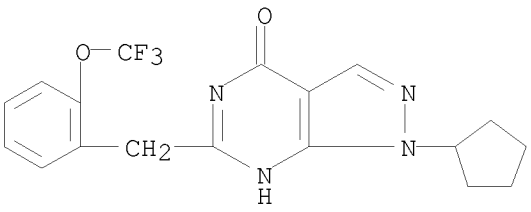

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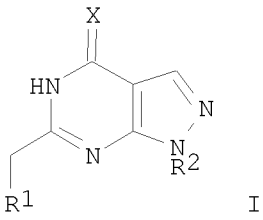

I

AB Title compds. (I; R1 = Ph substituted by 1-5 halo, alkyl, CF3, OCF3, cyano, OH, NO2, alkoxy; R2 = pentan-3-yl, C4-6 cycloalkyl; X = O, S), were prepared for improvement of perception, concentration, learning and/or memory (no data). Thus, 5-amino-1-cyclopentyl-1H-pyrazole-4-carboxamide (preparation given) and Et 3-chlorophenylacetate in EtOH at 0° were treated slowly with NaH followed by slow warming and then 18 h reflux to give 81% 6-(3-chlorobenzyl)-1-cyclopentyl-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:177919 CAPLUS
DOCUMENT NUMBER: 140:235735
TITLE: Preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.
INVENTOR(S): Hendrix, Martin; Boess, Frank-Gerhard; Burkhardt, Nils; Erb, Christina; Tersteegen, Adrian; Van Kampen, Marja
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 28 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10238724	A1	20040304	DE 2002-10238724	20020823
CA 2496308	A1	20040401	CA 2003-2496308	20030813
WO 2004026876	A1	20040401	WO 2003-EP8979	20030813
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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AU 2003251706	A1	20040408	AU 2003-251706	20030813
EP 1534713	A1	20050601	EP 2003-797239	20030813
EP 1534713	B1	20060111		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006503051	T	20060126	JP 2004-536941	20030813
ES 2256797	T3	20060716	ES 2003-797239	20030813
US 20060111372	A1	20060525	US 2005-524956	20051215
PRIORITY APPLN. INFO.:			DE 2002-10238724 A	20020823
			WO 2003-EP8979 W	20030813

OTHER SOURCE(S): MARPAT 140:235735
IT 667400-78-4P 667400-79-5P 667870-10-2P
667870-11-3P 667870-12-4P 667870-13-5P
667870-14-6P 667870-15-7P 667870-16-8P
667870-17-9P 667870-18-0P 667870-19-1P
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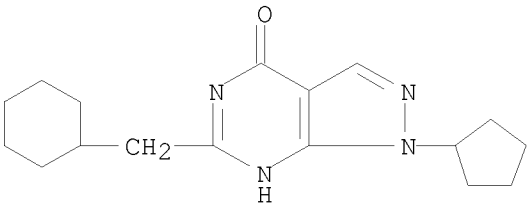
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.)
RN 667400-78-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(cyclohexylmethyl)-1-cyclopentyl-1,5-dihydro- (CA INDEX NAME)



RN 667400-79-5 CAPLUS
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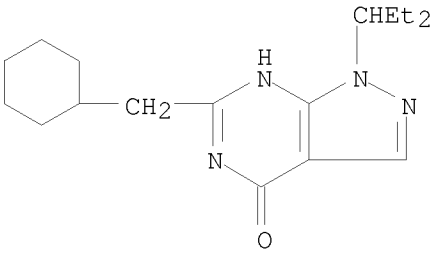
6-(cyclohexylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



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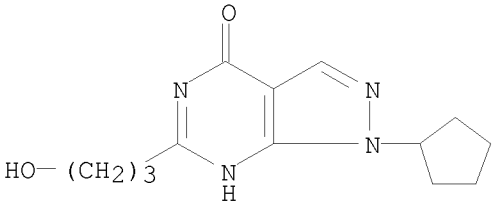

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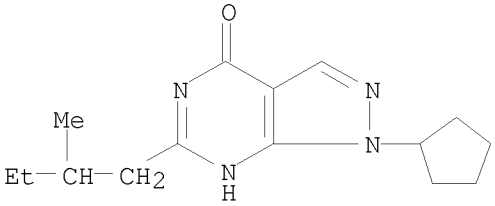

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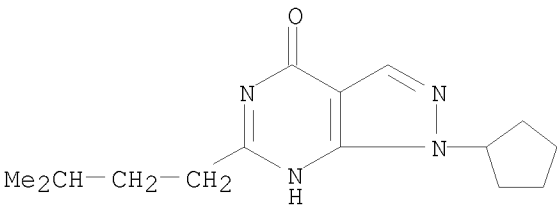

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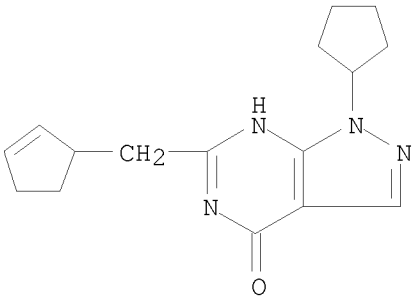

RN 667870-14-6 CAPLUS
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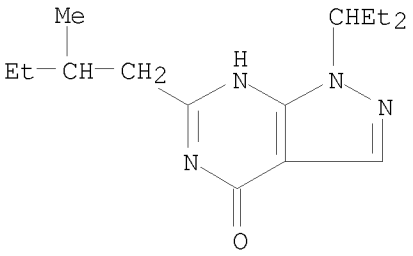
1-(1-ethylpropyl)-1,5-dihydro-6-(2-methylbutyl)- (CA INDEX NAME)



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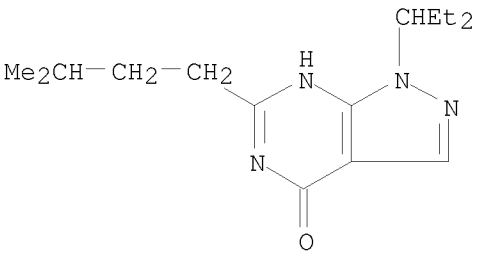

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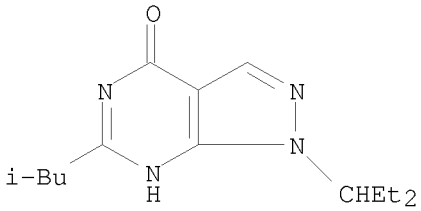
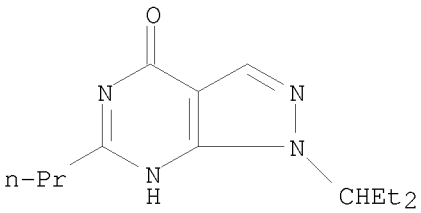


RN 667870-17-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-propyl-
(CA INDEX NAME)



RN 667870-18-0 CAPLUS
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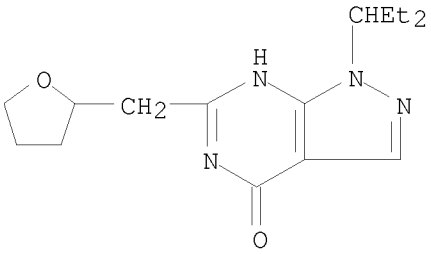
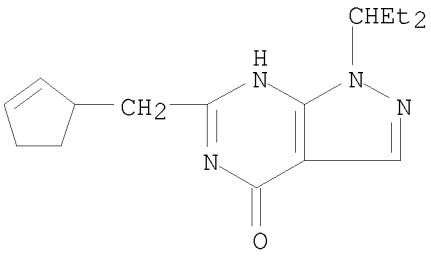
NAME)



RN 667870-19-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(2-cyclopenten-1-ylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



RN 667870-20-4 CAPLUS
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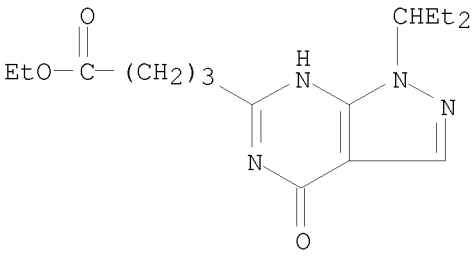
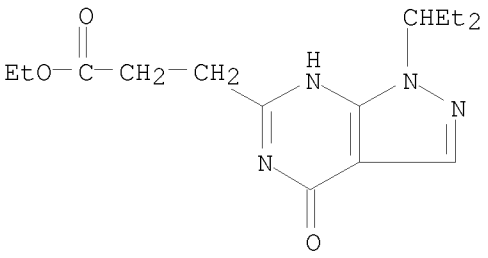
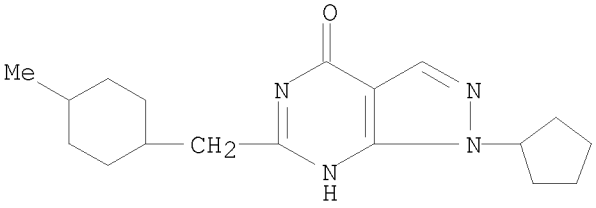


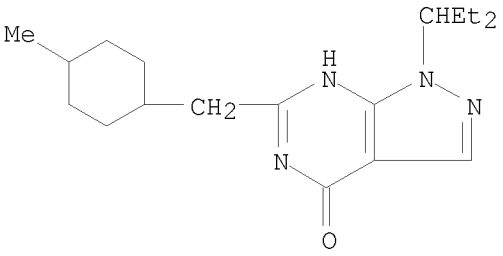
RN 667870-21-5 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid, 1-(1-ethylpropyl)-4,5-dihydro-4-oxo-, ethyl ester (CA INDEX NAME)



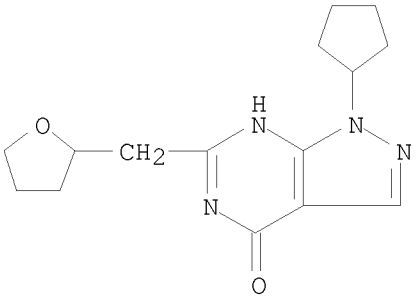
RN 667870-22-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(4-methylcyclohexyl)methyl]- (CA INDEX NAME)



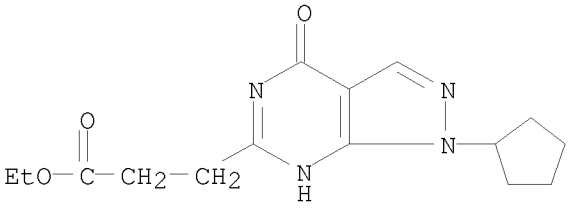
RN 667870-23-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylpropyl)-1,5-dihydro-6-[(4-methylcyclohexyl)methyl]- (CA INDEX NAME)



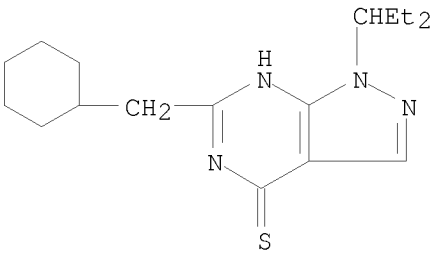
RN 667870-24-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-[(tetrahydro-2-furanyl)methyl]- (CA INDEX NAME)



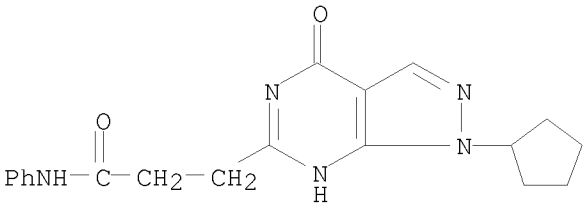
RN 667870-25-9 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid,
1-cyclopentyl-4,5-dihydro-4-oxo-, ethyl ester (CA INDEX NAME)



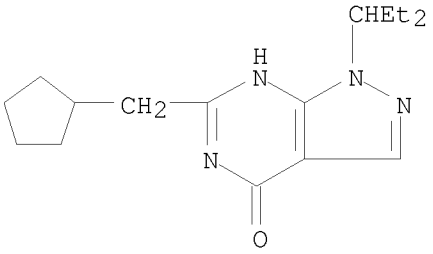
RN 667870-26-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione,
6-(cyclohexylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



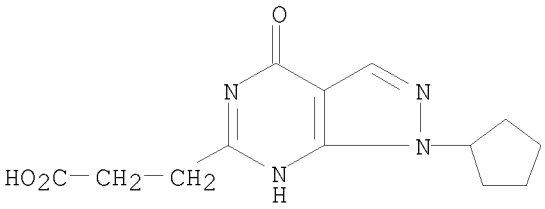
RN 667870-27-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanamide,
1-cyclopentyl-4,5-dihydro-4-oxo-N-phenyl- (CA INDEX NAME)



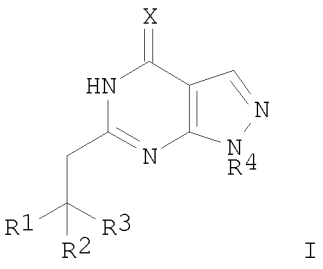
RN 667870-28-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(cyclopentylmethyl)-1-(1-ethylpropyl)-1,5-dihydro- (CA INDEX NAME)



IT 667870-31-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolopyrimidines as phosphodiesterase PDE9A inhibitors.)
RN 667870-31-7 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine-6-propanoic acid,
1-cyclopentyl-4,5-dihydro-4-oxo- (CA INDEX NAME)



GI



I

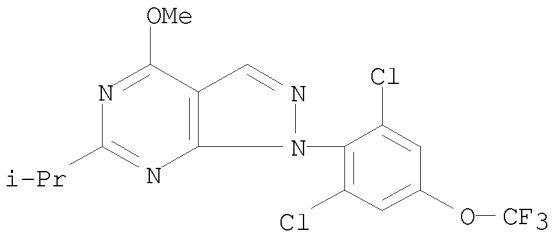
AB Title compds. [I; R1 = OH, (substituted) alkyl, alkoxy, CO2R5, CONR6R7; R5 = alkyl; R6, R7 = H, aryl, alkyl; NR6R7 = 4-10 membered heterocycle; R2 = H, alkyl, alkoxy; R3 = H, alkyl; R4 = pentan-3-yl, C4-6 cycloalkyl; X = O, S], were prepared Thus, 5-amino-1-cyclopentyl-1H-pyrazole-4-carboxamide (preparation given), Me cyclohexylacetate, and NaH were refluxed 18 h in EtOH to give 31% 6-cyclohexylmethyl-1-cyclopentyl-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one. The latter inhibited PDE9A with IC50 = 5 nM.

L4 ANSWER 21 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:891929 CAPLUS
DOCUMENT NUMBER: 139:381500
TITLE: Preparation of pyrazolo[3,4-d]pyrimidin-4-ones as herbicides and/or nematocides
INVENTOR(S): Linker, Karl-Heinz; Andree, Roland; Hoischen, Dorothee; Schwarz, Hans-Georg; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf; Loesel, Peter
PATENT ASSIGNEE(S): Bayer CropScience AG, Germany
SOURCE: Ger. Offen., 36 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

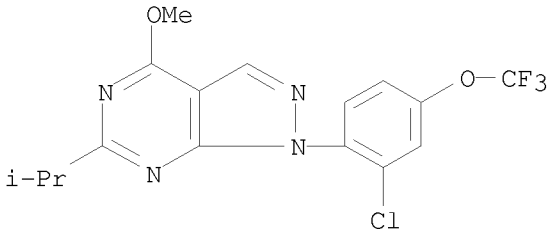
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10219435	A1	20031113	DE 2002-10219435	20020502
IN 2003MU00379	A	20050211	IN 2003-MU379	20030417
CA 2484997	A1	20031113	CA 2003-2484997	20030422
WO 2003093269	A2	20031113	WO 2003-EP4137	20030422
WO 2003093269	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003224111	A1	20031117	AU 2003-224111	20030422
EP 1504005	A2	20050209	EP 2003-720510	20030422
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003009873	A	20050426	BR 2003-9873	20030422
JP 2005531549	T	20051020	JP 2004-501408	20030422
US 20050209251	A1	20050922	US 2005-512834	20050519

PRIORITY APPLN. INFO.: DE 2002-10219435 A 20020502
WO 2003-EP4137 W 20030422

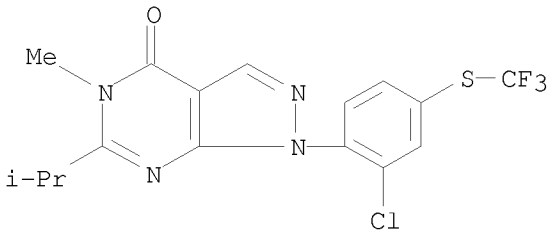
OTHER SOURCE(S): MARPAT 139:381500
IT 1053783-28-0 1053783-82-6 1053783-83-7
1053783-90-6 1053783-93-9 1053783-95-1
1053783-96-2
RL: PRPH (Prophetic)
(Preparation of pyrazolo[3,4-d]pyrimidin-4-ones as herbicides and/or nematocides)
RN 1053783-28-0 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethoxy)phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)



RN 1053783-82-6 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2-chloro-4-(trifluoromethoxy)phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)

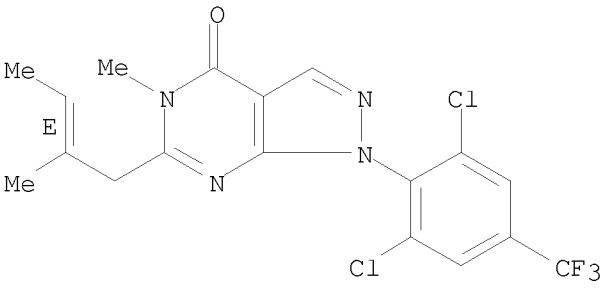


RN 1053783-83-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2-chloro-4-[(trifluoromethyl)thio]phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)

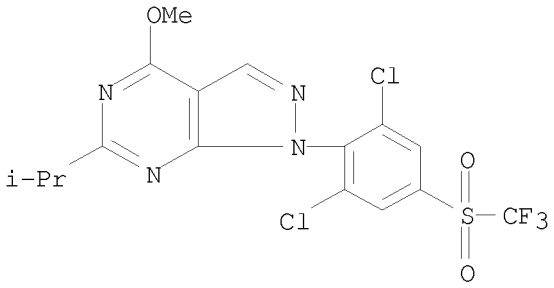


RN 1053783-90-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

Double bond geometry as shown.

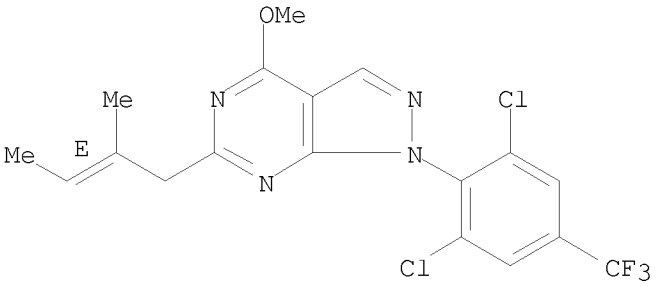


RN 1053783-93-9 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-[(trifluoromethyl)sulfonyl]phenyl]-4-methoxy-6-(1-methylethyl)- (CA INDEX NAME)

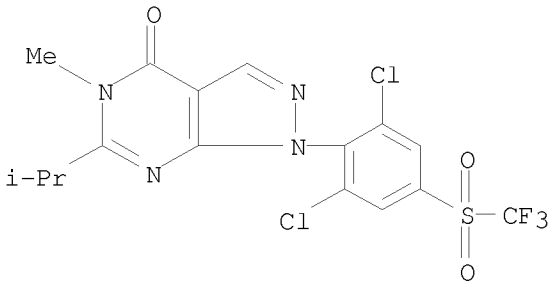


RN 1053783-95-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-methoxy-6-[(2E)-2-methyl-2-buten-1-yl]- (CA INDEX NAME)

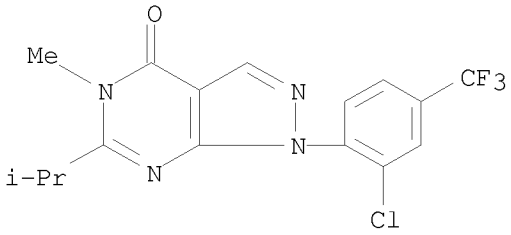
Double bond geometry as shown.



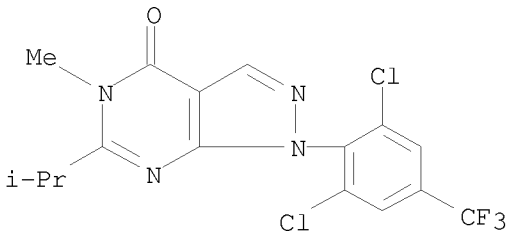
RN 1053783-96-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2,6-dichloro-4-[(trifluoromethyl)sulfonyl]phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



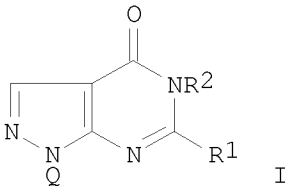
IT 623584-98-5P 623584-99-6P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidinones as herbicides and/or nematocides)
RN 623584-98-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2-chloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



RN 623584-99-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-1,5-dihydro-5-methyl-6-(1-methylethyl)- (CA INDEX NAME)



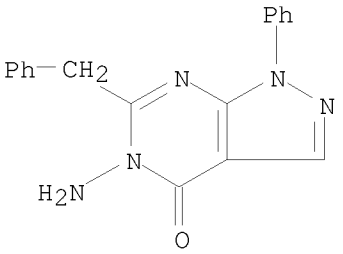
GI



I

AB Title compds. [I; Q = NO2, cyano, halo, (halogenated) alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, (hetero)aryl; R1 = H, (substituted) alkyl, alkoxycarbonyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, heterocyclyl; R2 = H, (substituted) alkyl, alkenyl, alkynyl], were prepared Thus, a mixture of 5-amino-1-(3-chloro-5-trifluoromethylpyridin-2-yl)pyrazole-4-carboxamide, CH(OMe)3, p-toluenesulfonic acid, and toluene was refluxed for 12 h followed by further addition of CH(OMe)3 and reflux for 12 h under stirring to give 44% 1-(3-chloro-5-trifluoromethylpyridin-2-yl)-1,5-dihydropyrazolo[3,4-d]pyrimidin-4-one. I were said to show very strong pre- and postemergent herbicidal activity, good crop tolerance, and good nematocidal activity.

L4 ANSWER 22 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:736859 CAPLUS
DOCUMENT NUMBER: 140:163756
TITLE: Design, synthesis, and antimicrobial activity of some new pyrazolo[3,4-d]pyrimidines
AUTHOR(S): Abdel-Gawad, Soad M.; Ghorab, M. M.; El-Sharief, A. M. Sh.; El-Telbany, F. A.; Abdel-Alla, M.
CORPORATE SOURCE: Department of Chemistry, Faculty of Science (Girl's), Al-Azhar University, Cairo, Egypt
SOURCE: Heteroatom Chemistry (2003), 14(6), 530-534
CODEN: HETCE8; ISSN: 1042-7163
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:163756
IT 654069-43-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(design, synthesis, and antibacterial activity of some new pyrazolo[3,4-d]pyrimidines from a phenylpyrazole carboxylate)
RN 654069-43-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



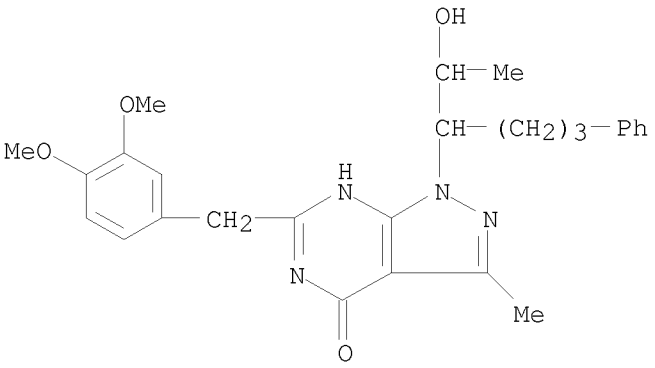
AB 2-Benzyl- and 2-aryloxymethyl-3-amino-1-phenyl-pyrazolo[3,4-d]pyrimidine-4-ones were synthesized by reacting arylacetylamino derivs. with hydrazine hydrate. Thionation of the above compds. by action of P2S5 in pyridine yielded 2-aryloxy-methyl-3-amino-1-phenyl-pyrazolo[3,4-d]pyrimidin-4-thiones. 2,5-Diphenyl-2,3-dihydro-1H-pyrazolo[5',1':4:5]-pyrazolo[3,4-d]pyrimidine-8-one was also obtained via reaction of ethyl-2-cinnamoylamino-1-phenyl-pyrazole-4-car-boxylate with hydrazine hydrate. The prepared compds. were screened in vitro for their antimicrobial activity. Some of the tested compds. were found to be active at 100 μg/mL compared with reference compds. (Ampicillin and Trivid) as antibacterial agents and claforan as antifungal agent.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:107116 CAPLUS
DOCUMENT NUMBER: 136:145267
TITLE: Selective phosphodiesterase 2 inhibitors used as medicaments for improving cognition
INVENTOR(S): Boss, Frank-Gerhard; Hendrix, Martin; Konig, Gerhard; Niewohner, Ulrich; Schlemmer, Karl-Heinz; Schreiber, Rudy; Van Der Staay, Franz-Josef; Schauss, Dagmar
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002009713	A2	20020207	WO 2001-EP8609	20010719
WO 2002009713	A3	20020718		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10122893	A1	20020321	DE 2001-10122893	20010511
CA 2417631	A1	20030129	CA 2001-2417631	20010719
EP 1307201	A2	20030507	EP 2001-969511	20010719
EP 1307201	B1	20041124		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004505054	T	20040219	JP 2002-515266	20010719
ES 2233685	T3	20050616	ES 2001-969511	20010719
US 20020132754	A1	20020919	US 2001-911277	20010723
US 7022709	B2	20060404		

PRIORITY APPLN. INFO.:
DE 2000-10037411 A 20000801
DE 2001-10122893 A 20010511
WO 2001-EP8609 W 20010719

OTHER SOURCE(S): MARPAT 136:145267
IT 213324-52-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(selective phosphodiesterase 2 inhibitors for improving cognition)
RN 213324-52-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]-3-methyl- (CA INDEX NAME)



AB The invention discloses the use of selective phosphodiesterase 2 inhibitors for producing medicaments to improve cognition, powers of concentration, learning capability, and/or memory retention.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:621218 CAPLUS
DOCUMENT NUMBER: 129:260471
ORIGINAL REFERENCE NO.: 129:53085a,53088a
TITLE: Preparation of pyrazolo[3,4-d]pyrimidinones as phosphodiesterase inhibitors
INVENTOR(S): Haning, Helmut; Niewohner, Ulrich; Rosentreter, Ulrich; Schenke, Thomas; Keldenich, Jorg; Bischoff, Erwin; Schlemmer, Karl-Heinz; Schutz, Helmuth; Thomas, Gunter
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9840384	A1	19980917	WO 1998-EP1086	19980226
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19709877	A1	19980917	DE 1997-19709877	19970311
CA 2283211	A1	19980917	CA 1998-2283211	19980226
AU 9868240	A	19980929	AU 1998-68240	19980226
AU 727615	B2	20001214		
EP 973774	A1	20000126	EP 1998-913595	19980226
EP 973774	B1	20030122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9807995	A	20000308	BR 1998-7995	19980226
NZ 337724	A	20000825	NZ 1998-337724	19980226
HU 2000001805	A2	20001128	HU 2000-1805	19980226
HU 2000001805	A3	20020930		
JP 2001514638	T	20010911	JP 1998-539135	19980226
AT 231509	T	20030215	AT 1998-913595	19980226
ES 2191294	T3	20030901	ES 1998-913595	19980226
RU 2219180	C2	20031220	RU 1999-121518	19980226
CN 1151155	C	20040526	CN 1998-804987	19980226
US 6174884	B1	20010116	US 1999-367538	19990816
MX 9908179	A	20000228	MX 1999-8179	19990906
HK 1028035	A1	20050318	HK 2000-107378	20001117

PRIORITY APPLN. INFO.: DE 1997-19709877 A 19970311
WO 1998-EP1086 W 19980226

OTHER SOURCE(S): MARPAT 129:260471
IT 213324-17-5P 213324-18-6P 213324-19-7P
213324-20-0P 213324-21-1P 213324-22-2P
213324-23-3P 213324-24-4P 213324-25-5P
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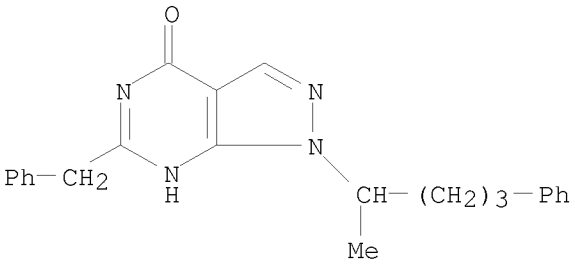
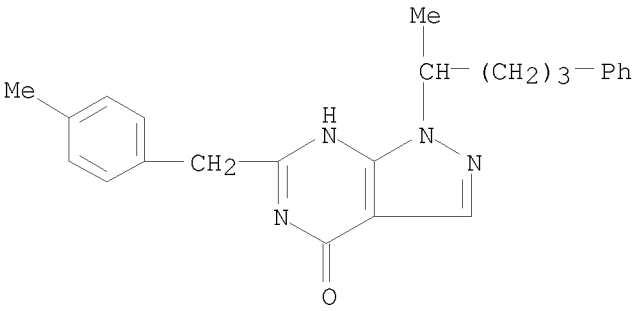
213324-77-7P 213324-78-8P 213324-81-3P
213324-82-4P 213324-83-5P 213324-84-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolo[3,4-d]pyrimidinones as phosphodiesterase inhibitors)

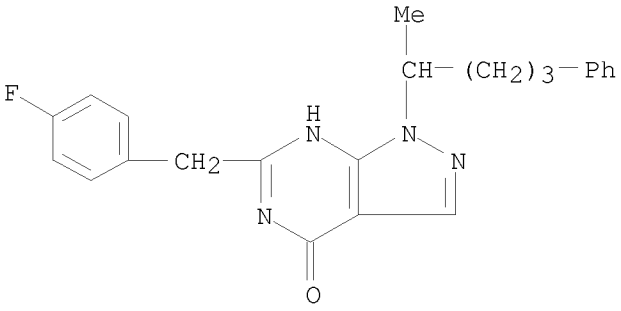
RN 213324-17-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-methyl-4-phenylbutyl)-6-(phenylmethyl)- (CA INDEX NAME)



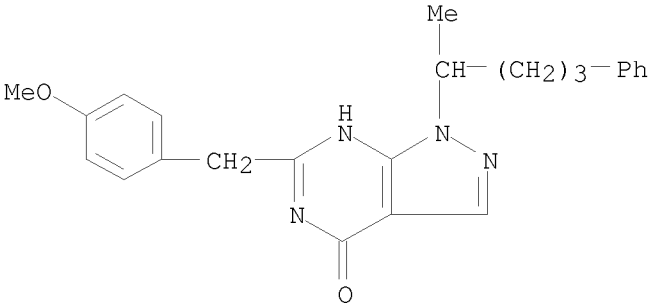
RN 213324-18-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-methyl-4-phenylbutyl)-6-[(4-methylphenyl)methyl]- (CA INDEX NAME)



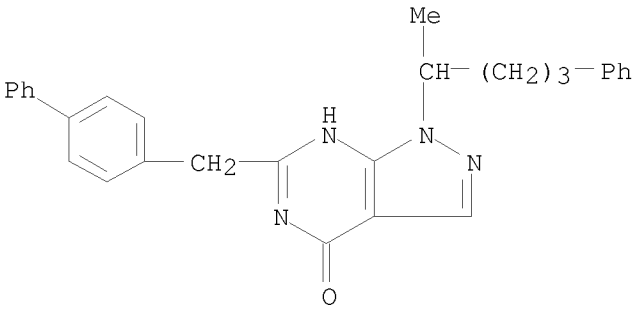
RN 213324-19-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(4-fluorophenyl)methyl]-1,5-dihydro-1-(1-methyl-4-phenylbutyl)- (CA INDEX NAME)



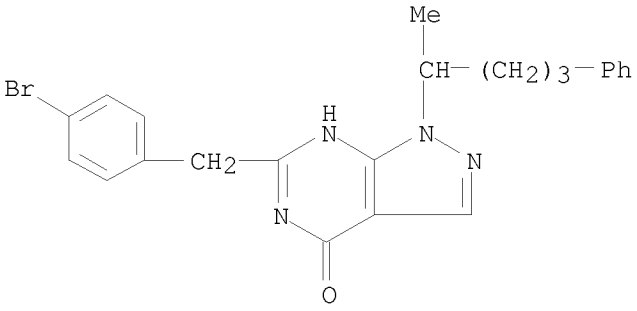
RN 213324-20-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(4-methoxyphenyl)methyl]-1-(1-methyl-4-phenylbutyl)- (CA INDEX NAME)



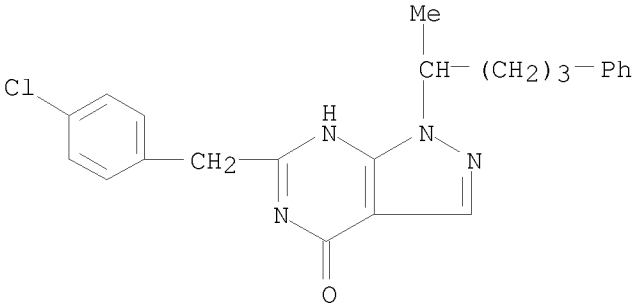
RN 213324-21-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-([1,1'-biphenyl]-4-ylmethyl)-1,5-dihydro-1-(1-methyl-4-phenylbutyl)- (CA INDEX NAME)



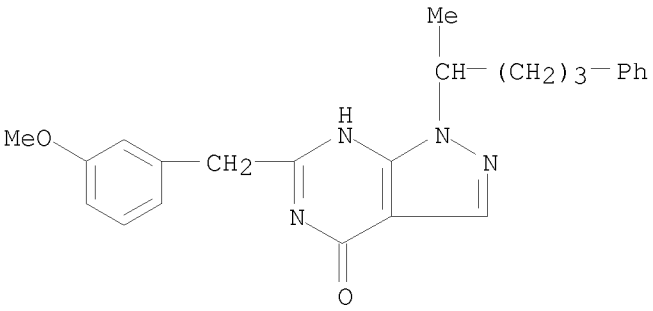
RN 213324-22-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(4-bromophenyl)methyl]-1,5-dihydro-1-(1-methyl-4-phenylbutyl)- (CA INDEX NAME)



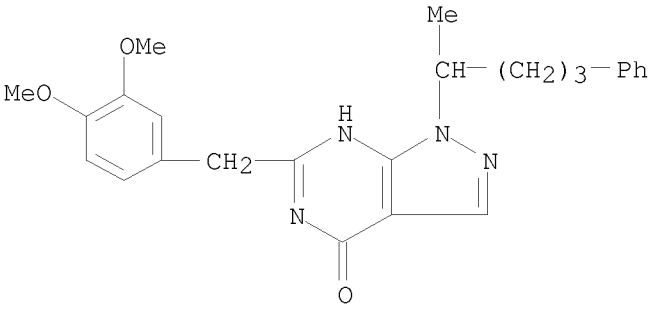
RN 213324-23-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(4-chlorophenyl)methyl]-1,5-dihydro-1-(1-methyl-4-phenylbutyl)- (CA INDEX NAME)



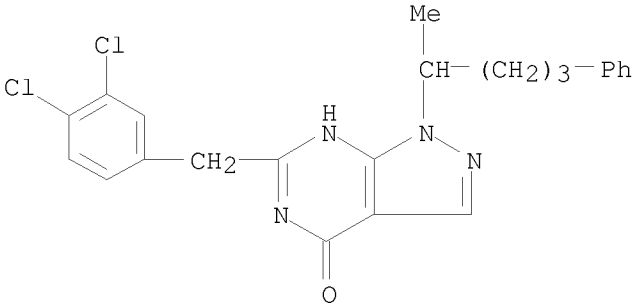
RN 213324-24-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(3-methoxyphenyl)methyl]-1-(1-methyl-4-phenylbutyl)- (CA INDEX NAME)



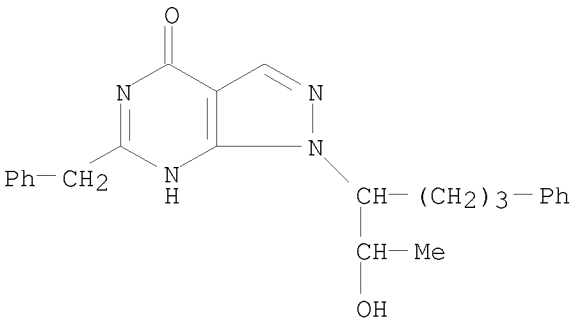
RN 213324-25-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-1-(1-methyl-4-phenylbutyl)- (CA INDEX NAME)



RN 213324-26-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3,4-dichlorophenyl)methyl]-1,5-dihydro-1-(1-methyl-4-phenylbutyl)-
(CA INDEX NAME)

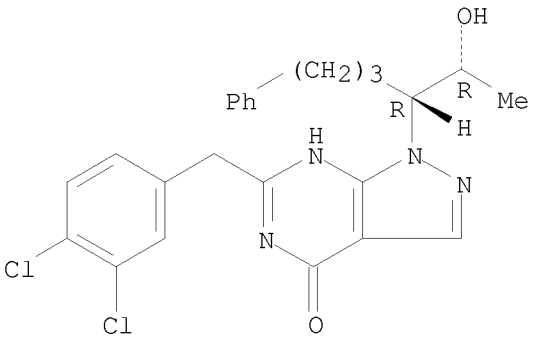


RN 213324-29-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]-6-(phenylmethyl)- (CA
INDEX NAME)



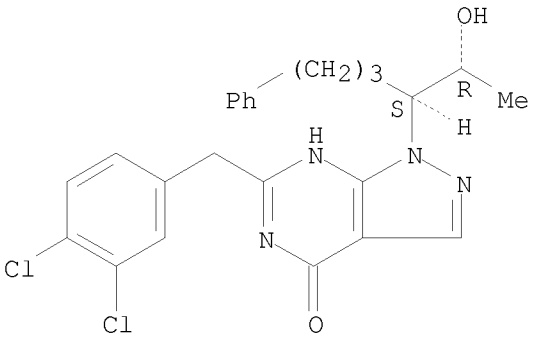
RN 213324-30-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3,4-dichlorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-
4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



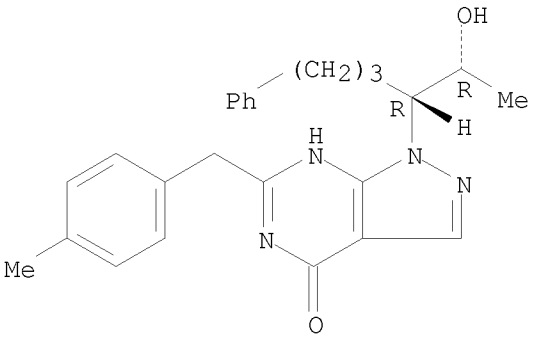
RN 213324-31-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3,4-dichlorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-
4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



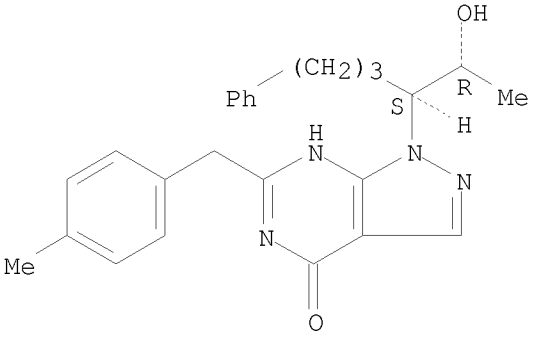
RN 213324-32-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-4-phenylbutyl]-6-[(4-
methylphenyl)methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

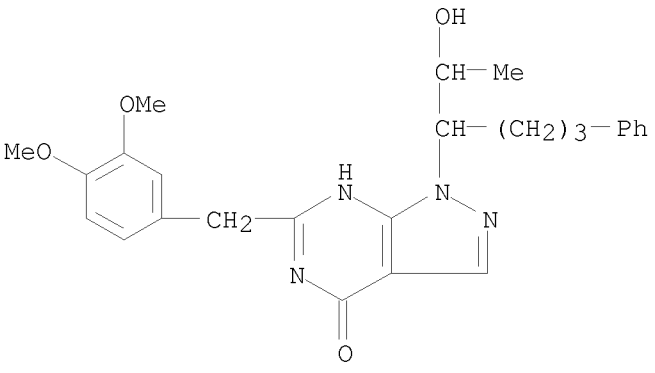


RN 213324-33-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-6-[(4-methylphenyl)methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

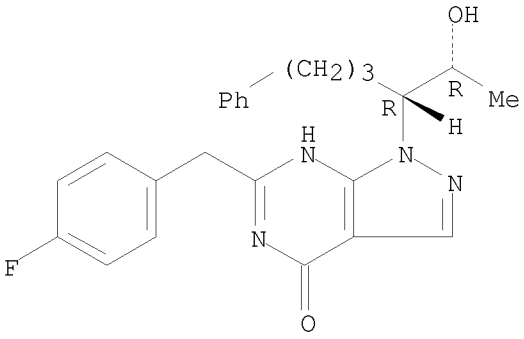


RN 213324-34-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]- (CA INDEX NAME)



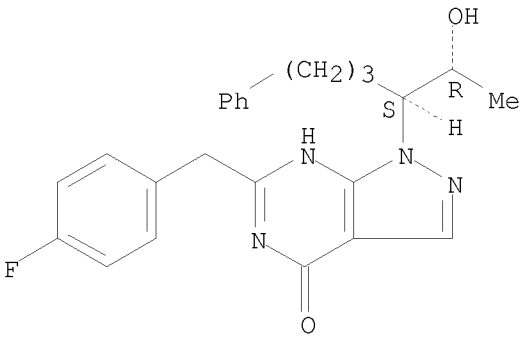
RN 213324-35-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-fluorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



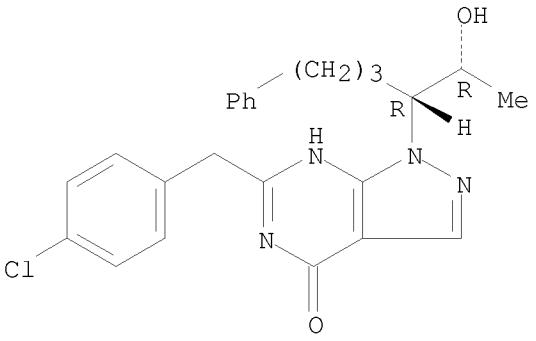
RN 213324-36-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-fluorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



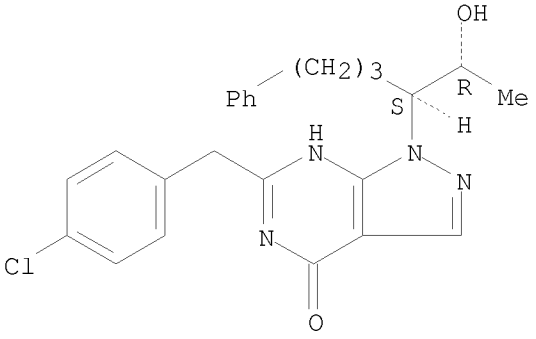
RN 213324-37-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-chlorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



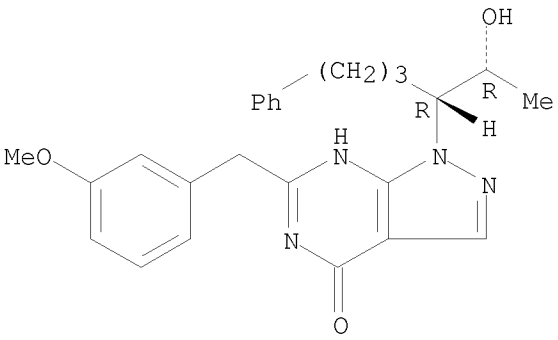
RN 213324-38-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(4-chlorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



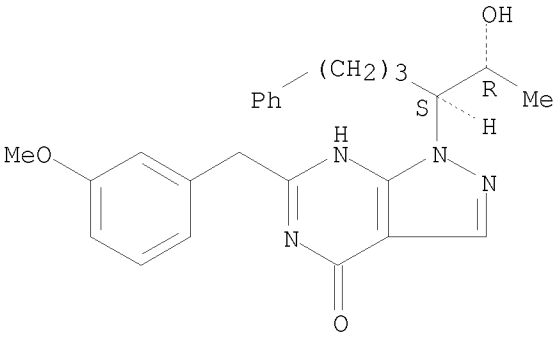
RN 213324-39-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-4-phenylbutyl]-6-[(3-methoxyphenyl)methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



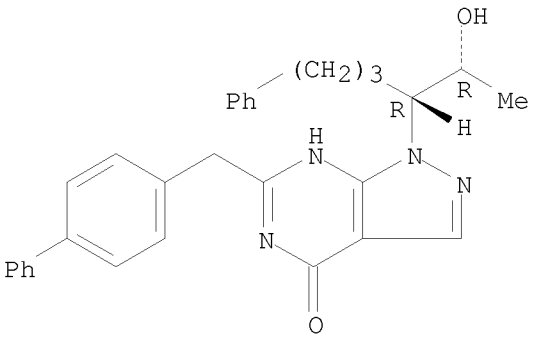
RN 213324-40-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-6-[(3-
methoxyphenyl)methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



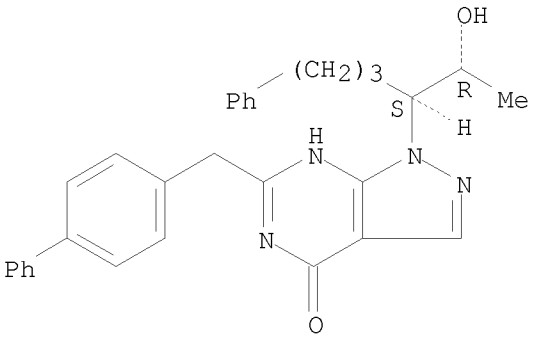
RN 213324-41-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-([1,1'-biphenyl]-4-ylmethyl)-1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-
4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



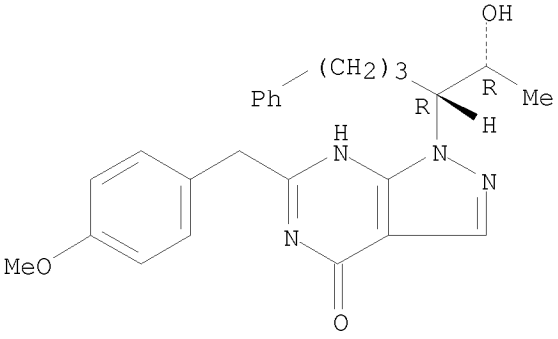
RN 213324-42-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-([1,1'-biphenyl]-4-ylmethyl)-1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-
4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



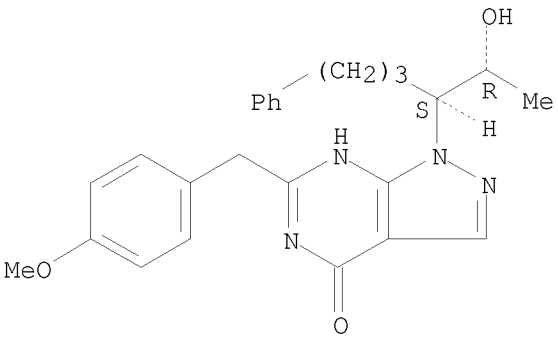
RN 213324-43-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-4-phenylbutyl]-6-[(4-methoxyphenyl)methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



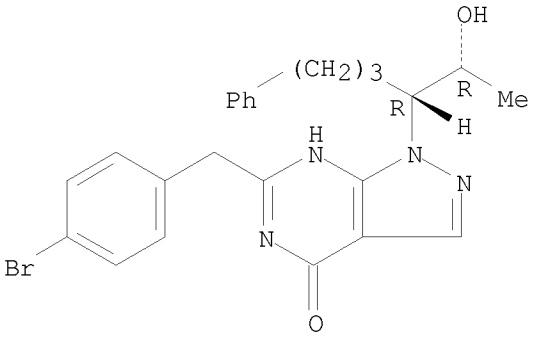
RN 213324-44-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-6-[(4-methoxyphenyl)methyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



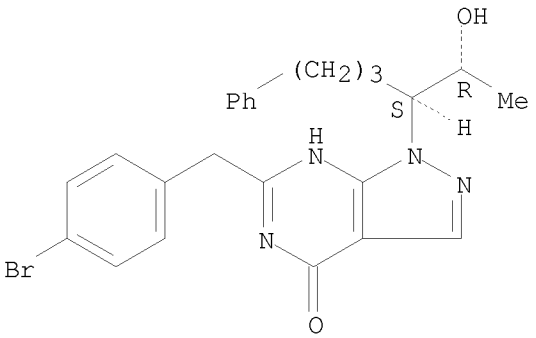
RN 213324-45-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-bromophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

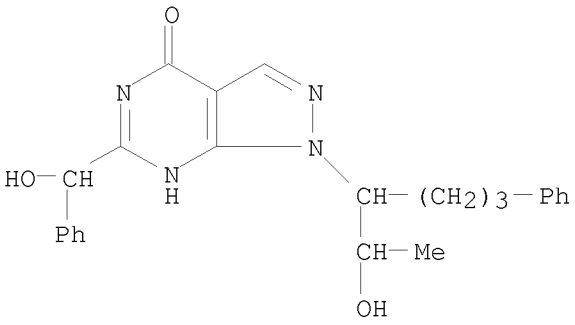


RN 213324-46-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-bromophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

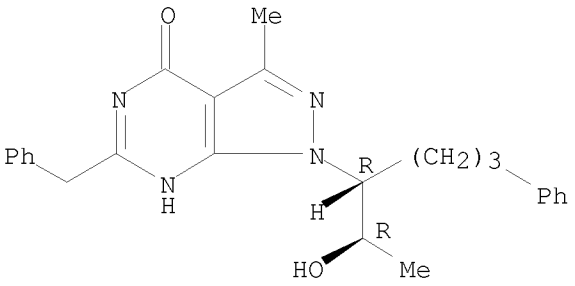


RN 213324-47-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]-6-(hydroxyphenylmethyl)-
(CA INDEX NAME)



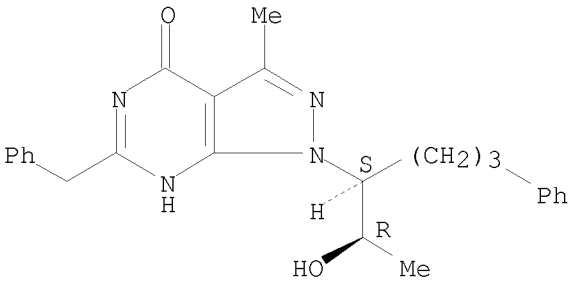
RN 213324-48-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-4-phenylbutyl]-3-methyl-6-
(phenylmethyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



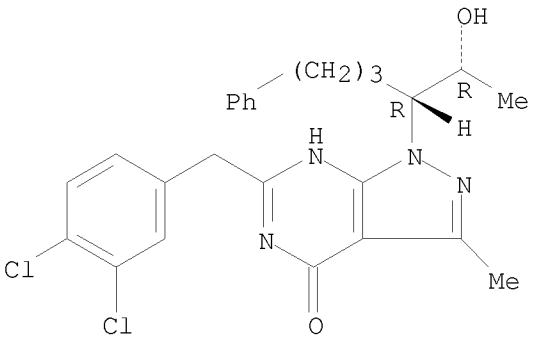
RN 213324-49-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-3-methyl-6-
(phenylmethyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



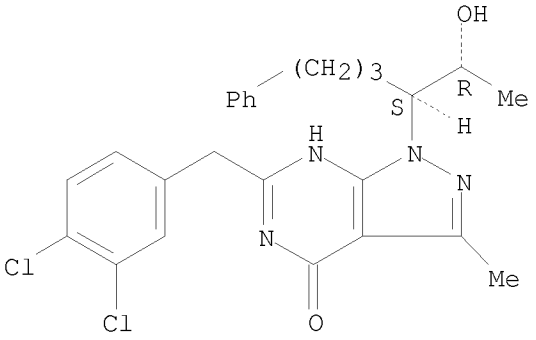
RN 213324-50-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3,4-dichlorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1R)-1-hydroxyethyl]-
4-phenylbutyl]-3-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.

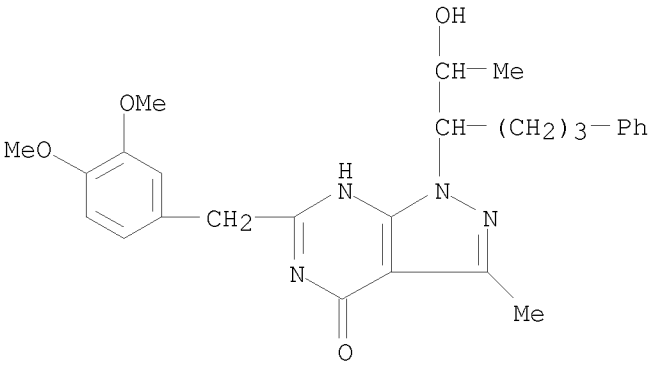


RN 213324-51-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3,4-dichlorophenyl)methyl]-1,5-dihydro-1-[(1R)-1-[(1S)-1-hydroxyethyl]-4-phenylbutyl]-3-methyl-, rel- (CA INDEX NAME)

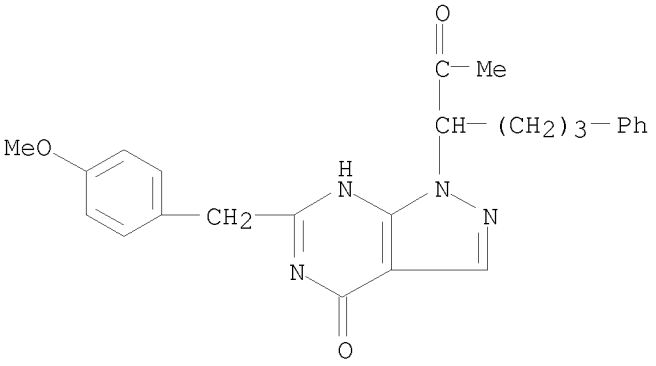
Relative stereochemistry.



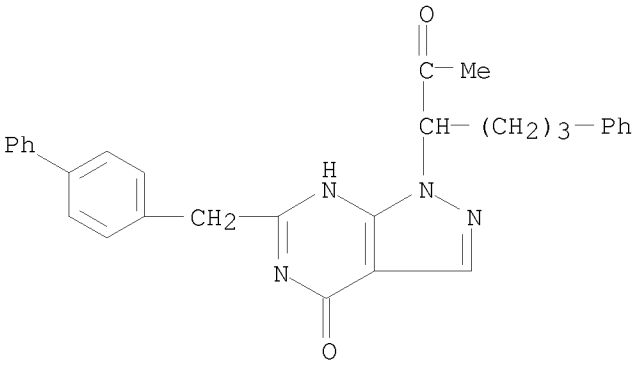
RN 213324-52-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]-3-methyl- (CA INDEX NAME)



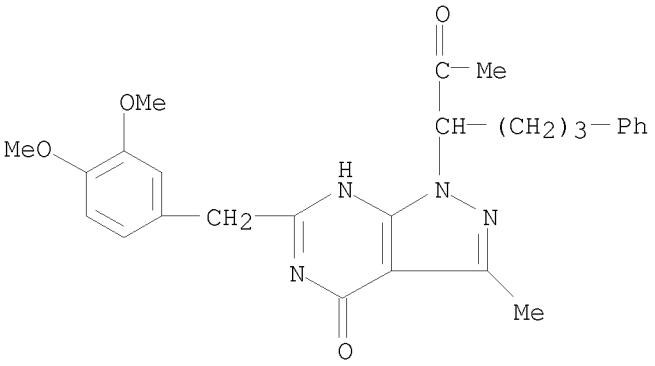
RN 213324-53-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-acetyl-4-phenylbutyl)-1,5-dihydro-6-[(4-methoxyphenyl)methyl]- (CA INDEX NAME)



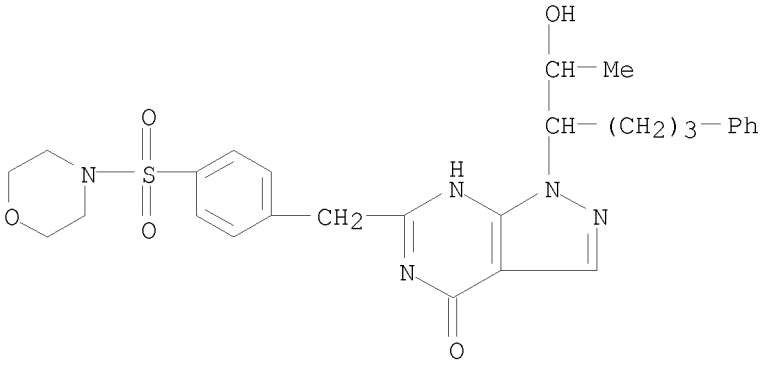
RN 213324-54-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-acetyl-4-phenylbutyl)-6-([1,1'-biphenyl]-4-ylmethyl)-1,5-dihydro- (CA INDEX NAME)



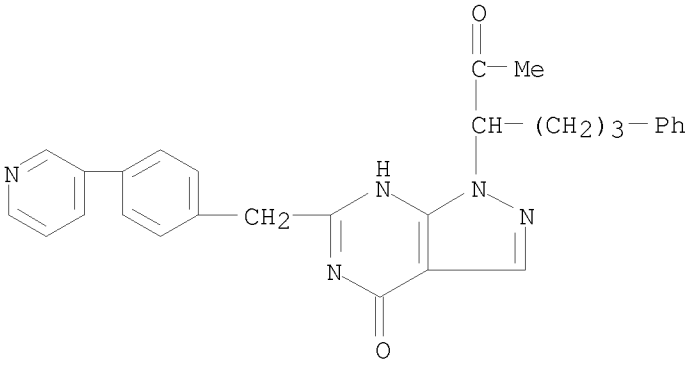
RN 213324-55-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-acetyl-4-phenylbutyl)-6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-3-methyl- (CA INDEX NAME)



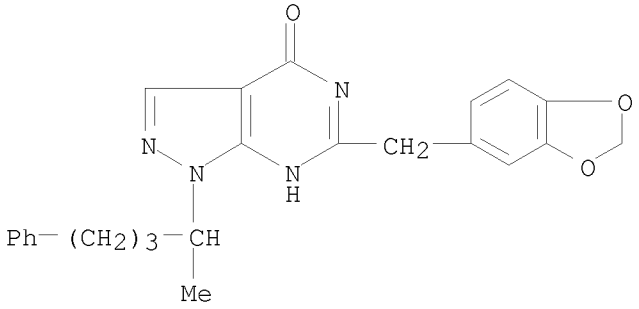
RN 213324-56-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-[1-(1-hydroxyethyl)-4-phenylbutyl]-6-[[4-(4-morpholinylsulfonyl)phenyl]methyl]- (CA INDEX NAME)



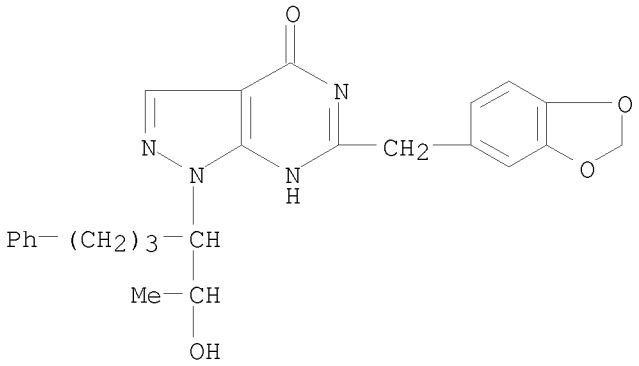
RN 213324-57-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-acetyl-4-phenylbutyl)-1,5-dihydro-6-[[4-(3-pyridinyl)phenyl]methyl]- (CA INDEX NAME)



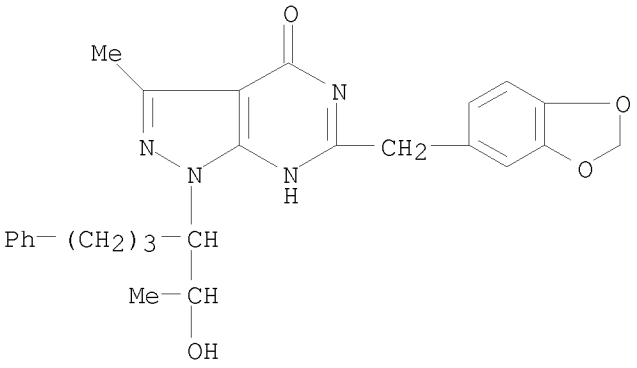
RN 213324-62-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(1,3-benzodioxol-5-ylmethyl)-1,5-dihydro-1-(1-methyl-4-phenylbutyl)-
(CA INDEX NAME)



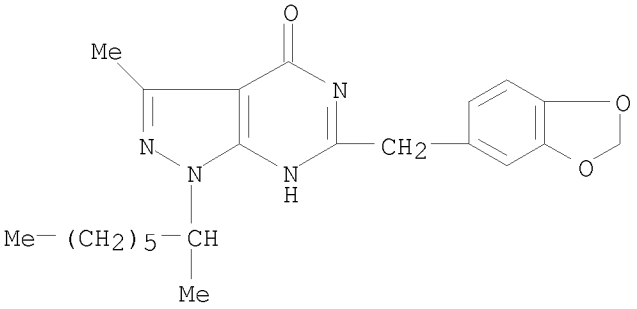
RN 213324-68-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(1,3-benzodioxol-5-ylmethyl)-1,5-dihydro-1-[1-(1-hydroxyethyl)-4-
phenylbutyl]- (CA INDEX NAME)



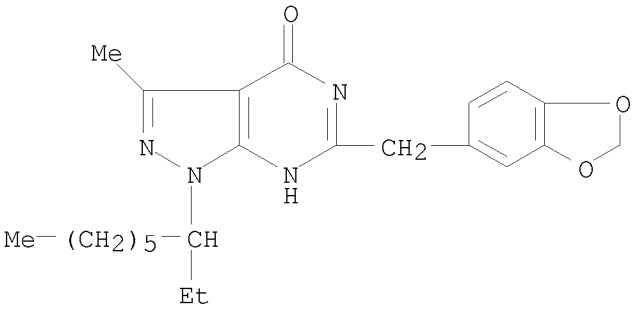
RN 213324-69-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(1,3-benzodioxol-5-ylmethyl)-1,5-dihydro-1-[1-(1-hydroxyethyl)-4-
phenylbutyl]-3-methyl- (CA INDEX NAME)



RN 213324-70-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(1,3-benzodioxol-5-ylmethyl)-1,5-dihydro-3-methyl-1-(1-methylheptyl)-
(CA INDEX NAME)

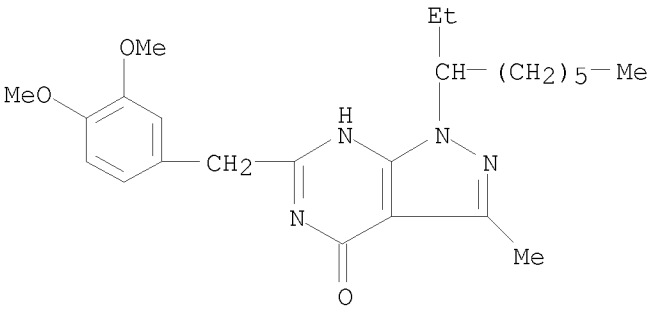


RN 213324-72-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(1,3-benzodioxol-5-ylmethyl)-1-(1-ethylheptyl)-1,5-dihydro-3-methyl-
(CA INDEX NAME)

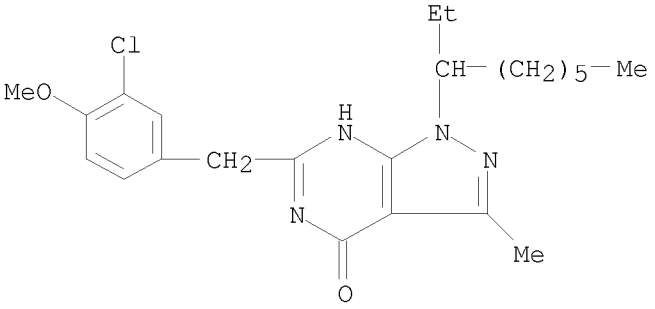


RN 213324-73-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3,4-dimethoxyphenyl)methyl]-1-(1-ethylheptyl)-1,5-dihydro-3-methyl-

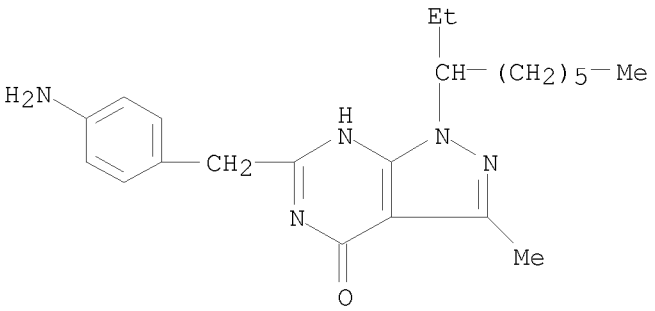
(CA INDEX NAME)



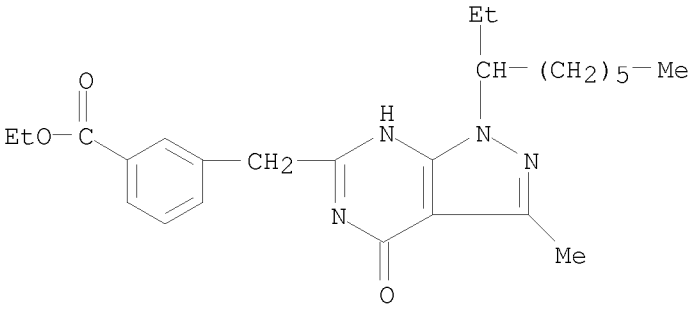
RN 213324-74-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(3-chloro-4-methoxyphenyl)methyl]-1-(1-ethylheptyl)-1,5-dihydro-3-methyl- (CA INDEX NAME)



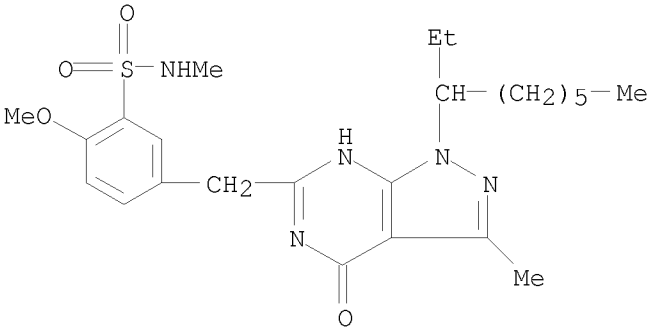
RN 213324-75-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(4-aminophenyl)methyl]-1-(1-ethylheptyl)-1,5-dihydro-3-methyl- (CA INDEX NAME)



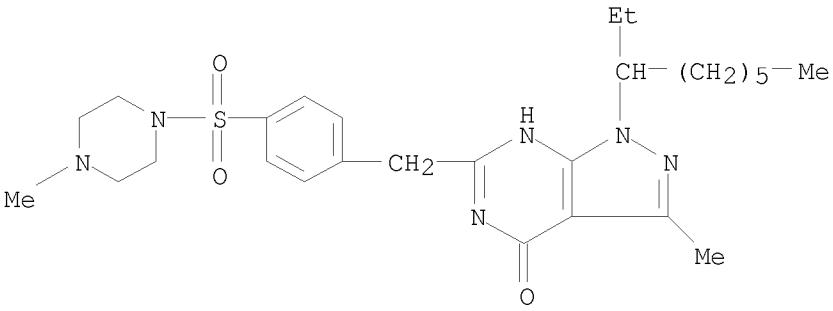
RN 213324-76-6 CAPLUS
CN Benzoic acid, 3-[[1-(1-ethylheptyl)-4,5-dihydro-3-methyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl]methyl]-, ethyl ester (CA INDEX NAME)



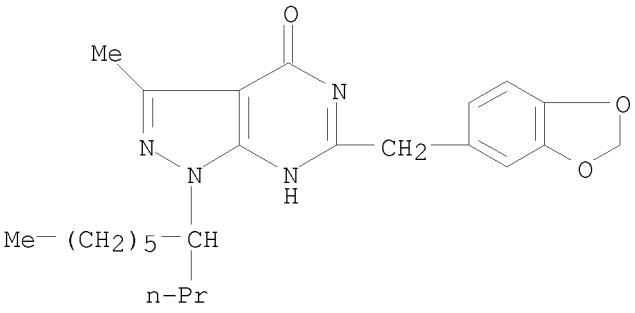
RN 213324-77-7 CAPLUS
CN Benzenesulfonamide, 5-[[1-(1-ethylheptyl)-4,5-dihydro-3-methyl-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-6-yl]methyl]-2-methoxy-N-methyl- (CA INDEX NAME)



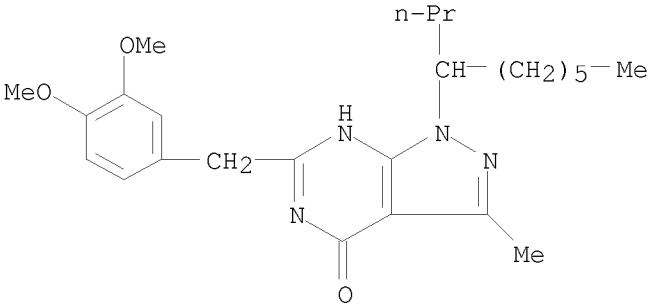
RN 213324-78-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1-ethylheptyl)-1,5-dihydro-3-methyl-6-[[4-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]methyl]- (CA INDEX NAME)



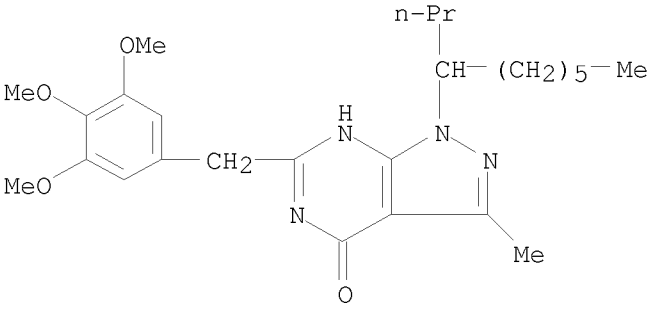
RN 213324-81-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(1,3-benzodioxol-5-ylmethyl)-1,5-dihydro-3-methyl-1-(1-propylheptyl)- (CA INDEX NAME)



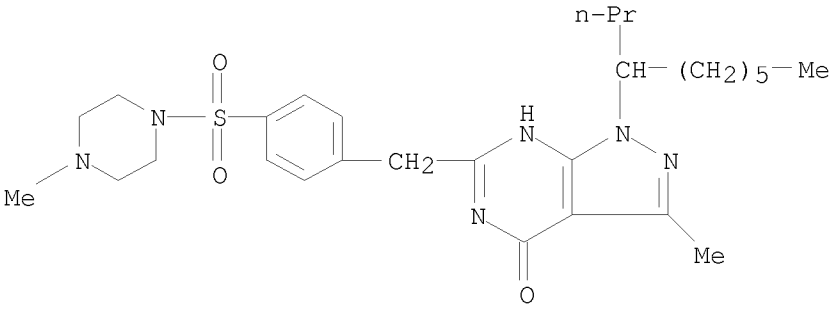
RN 213324-82-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(3,4-dimethoxyphenyl)methyl]-1,5-dihydro-3-methyl-1-(1-propylheptyl)-
(CA INDEX NAME)



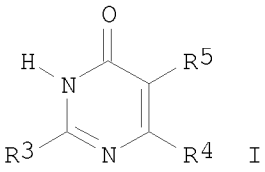
RN 213324-83-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-3-methyl-1-(1-propylheptyl)-6-[(3,4,5-trimethoxyphenyl)methyl]-
(CA INDEX NAME)



RN 213324-84-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-3-methyl-6-[[4-[(4-methyl-1-
piperazinyl)sulfonyl]phenyl]methyl]-1-(1-propylheptyl)- (CA INDEX NAME)



GI



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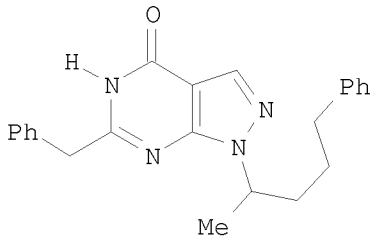
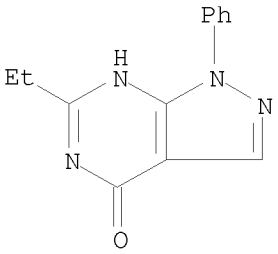


II

AB Title compds. [I; R3 = EL; E = (hydroxy)alk(en)ylene or CO; R4 = NRCHR1TV; L,V = aryl or heterocyclyl; RR5 = N:CR2 or NHCO; R1 = (un)substituted alkyl or acyl; R2 = H, cyano, alkoxy(carbonyl), etc.; T = CH2XY; X = bond, O, S, NH; Y = alkylene] were prepared Thus, MeCO(CH2)3Ph was condensed with H2NNHCO2CMe3 and the reduced product cyclocondensed with EtOCH:C(CN)2 to give 5-amino-1-(5-phenyl-2-pentyl)-1H-pyrazole-4-carbonitrile which was cyclocondensed with PhCH2COCl to give title compound II. Data for biol. activity of I were given.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:226504 CAPLUS
DOCUMENT NUMBER: 128:282737
ORIGINAL REFERENCE NO.: 128:55970h,55971a
TITLE: Catalytic action of azolium salts. IX. Synthesis of 6-aroyl-9H-purines and their analogs by nucleophilic aroylation catalyzed by imidazolium or benzimidazolium salt
AUTHOR(S): Miyashita, Akira; Suzuki, Yumiko; Iwamoto, Ken-Ichi; Higashino, Takeo
CORPORATE SOURCE: School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, 422, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1998), 46(3), 390-399
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:282737
IT 5394-42-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 6-aroyl-9H-purines and analogs via nucleophilic aroylation catalyzed by imidazolium or benzimidazolium salt)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



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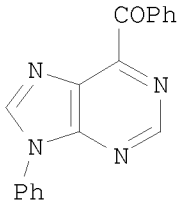


II

AB In the presence of 1,3-dimethylimidazolium iodide (I), 6-chloro-9-phenyl-9H-purine and 4-chloro-5,6-dimethylpyrrolo[2,3-d]pyrimidines underwent nucleophilic aroylation with arenecarbaldehydes to give the corresponding fused aroylpyrimidines, e.g. II. 1,3-Dimethylbenzimidazolium iodide (III) was an effective catalyst for the

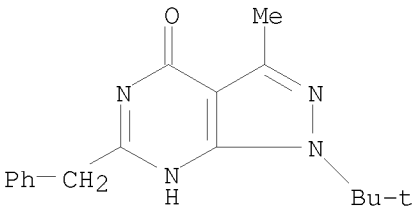
similar synthesis of 7-aroyl-3-phenyl-3H-1,2,3-triazolo[4,5-d]pyrimidines. In the synthesis of 4-aroyl-1H-pyrazolo[3,4-d]pyrimidines, both azolium salts I and III were effective as catalysts. Moreover, 4-aroyl-7H-pyrrolo[2,3-d]pyrimidines were obtained in good yields via the 4-tosyl derivs., in the presence of catalytic amts. of sodium p-toluenesulfinate and the imidazolium salt I. This catalytic aroylation was found to be a facile and useful method for the synthesis of 6-aroyl-9H-purines and their analogs.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

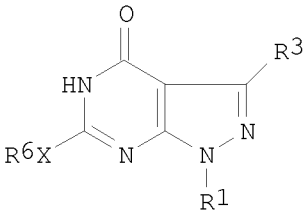
L4 ANSWER 26 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:664939 CAPLUS
DOCUMENT NUMBER: 125:301016
ORIGINAL REFERENCE NO.: 125:56346h,56347a
TITLE: 6-Substituted pyrazolo[3,4-d]pyrimidin-4-ones and compositions and methods of use as c-GMP phosphodiesterase inhibitors
INVENTOR(S): Bacon, Edward R.; Daum, Sol J.; Singh, Baldev
PATENT ASSIGNEE(S): Sanofi Winthrop, Inc., USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9628429	A1	19960919	WO 1996-US2971	19960305
W: AU, CA, CN, CZ, HU, JP, KR, MX, NO, NZ, PL, RU				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5656629	A	19970812	US 1995-402268	19950310
CA 2211669	A1	19960919	CA 1996-2211669	19960305
AU 9654188	A	19961002	AU 1996-54188	19960305
AU 708750	B2	19990812		
EP 813527	A1	19971229	EP 1996-911244	19960305
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1177960	A	19980401	CN 1996-192462	19960305
HU 9801336	A2	19981028	HU 1998-1336	19960305
HU 9801336	A3	20000728		
JP 11501923	T	19990216	JP 1996-527681	19960305
ZA 9601947	A	19961007	ZA 1996-1947	19960311
US 5977118	A	19991102	US 1997-824600	19970326
NO 9704151	A	19971104	NO 1997-4151	19970909
PRIORITY APPLN. INFO.:			US 1995-402268 A	19950310
			WO 1996-US2971 W	19960305

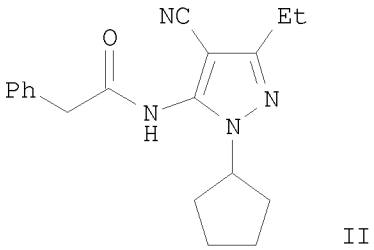
OTHER SOURCE(S): MARPAT 125:301016
IT 182879-50-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazolopyrimidinones as c-GMP phosphodiesterase inhibitors)
RN 182879-50-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(1,1-dimethylethyl)-1,5-dihydro-3-methyl-6-(phenylmethyl)- (CA INDEX NAME)



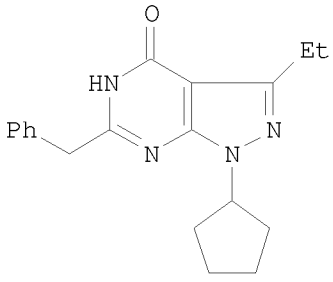
GI



I



II

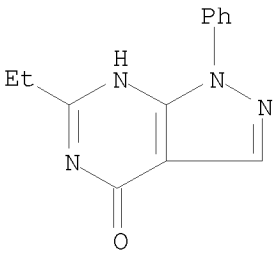


III

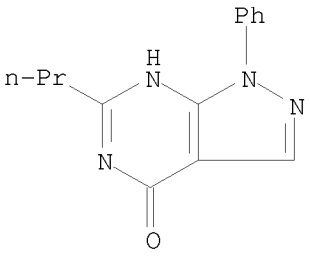
AB 6-Substituted pyrazolo[3,4-d]pyrimidin-4-one derivs. I [R1 = tert-Bu, cyclopentyl; R3 = Me, Et, PhCH2; X = CH2, O, NH; R6 = (un)substituted Ph, or (when X = CH2) OH or certain specified heterocyclic radicals] and their pharmaceutically acceptable salts or hydrates are claimed. Also claimed are pharmaceutical compns. containing them, and methods for their use in: (a) effecting c-GMP-phosphodiesterase inhibition, (b) treating heart failure and/or hypertension, (c) reversing or reducing nitrate-induced tolerance, and (d) treating angina pectoris, congestive heart disease, and myocardial infarction. Examples include 39 syntheses and 3 bioassays. For instance, 1-cyclopentyl-3-ethyl-5-amino-1H-pyrazole-4-carbonitrile underwent amidation with PhCH2COCl in pyridine to give 64% intermediate II, which underwent H2O2-mediated hydrolysis and cyclization in aqueous NaOH to give title compound III. At 1 mg/kg i.v. in spontaneously hypertensive rats, III gave a 15% redn in mean arterial pressure in 5 min. III had an IC50 of 10 nM for inhibition of c-GMP phosphodiesterase V in vitro.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

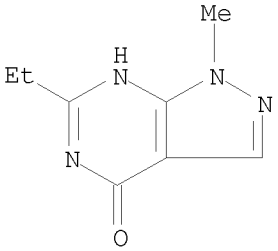
L4 ANSWER 27 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1992:174107 CAPLUS
DOCUMENT NUMBER: 116:174107
ORIGINAL REFERENCE NO.: 116:29471a,29474a
TITLE: Versatile synthesis of 6-alkyl(aryl)-1H-pyrazolo[3,4-d]pyrimidin-4[5H]-ones
AUTHOR(S): Reddy, K. Hemender; Reddy, A. Panduranga; Veeranagaiah, V.
CORPORATE SOURCE: Nizam Coll., Osmania Univ., Hyderabad, 500 001, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1992), 31B(3), 163-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:174107
IT 5394-42-3P 130925-64-3P 130925-68-7P
139954-52-2P 139954-53-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



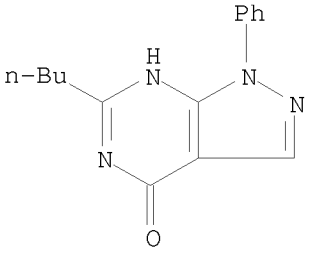
RN 130925-64-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA INDEX NAME)



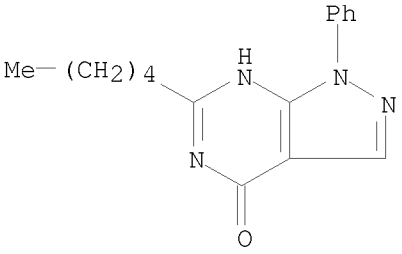
RN 130925-68-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl- (CA INDEX NAME)



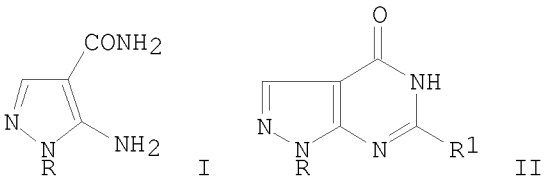
RN 139954-52-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-butyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



RN 139954-53-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-pentyl-1-phenyl- (CA INDEX NAME)



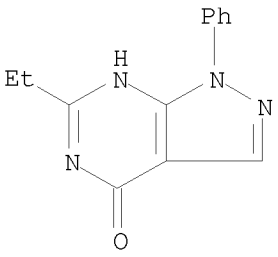
GI



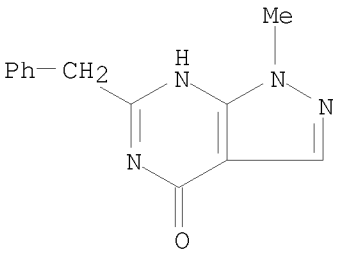
AB Condensation of 5-amino-1H-pyrazole-4-carboxamide (I, R = H) with various aromatic aldehydes furnishes 6-substituted

1H-pyrazole[3,4-d]pyrimidin-4(5H)-ones II (R1 = Ph, substituted Ph) via the intermediate 5-(N-arylideneamino)pyrazole-4-carboxamides. II were also synthesized by the reaction of I (R = H) with aromatic carboxylic acids in polyphosphoric acid (PPA) or polyphosphate ester (PPE). Similar treatment of I (R = Ph, Me) with aromatic aldehydes and aromatic carboxylic acids gives exclusively 6-substituted 1-methyl/phenyl-1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones. The title compds. have were also synthesized by the reaction of I with arylideneanilines.

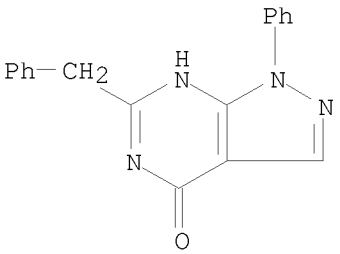
L4 ANSWER 28 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:6429 CAPLUS
DOCUMENT NUMBER: 114:6429
ORIGINAL REFERENCE NO.: 114:1267a,1270a
TITLE: Studies on pyrazolo[3,4-d]pyrimidine derivatives. XVIII. Facile preparation of 1H-pyrazolo[3,4-d]pyrimidin-4(5H)-ones
AUTHOR(S): Miyashita, Akira; Iijima, Chihoko; Higashino, Takeo; Matsuda, Hideaki
CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
SOURCE: Heterocycles (1990), 31(7), 1309-14
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:6429
IT 5394-42-3P 91803-32-6P 94331-62-1P
130925-64-3P 130925-65-4P 130925-68-7P
130925-69-8P 130925-70-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



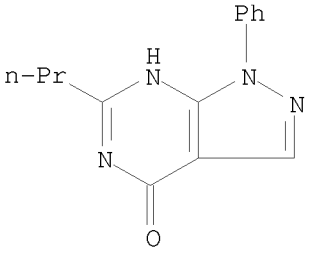
RN 91803-32-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(phenylmethyl)- (CA INDEX NAME)



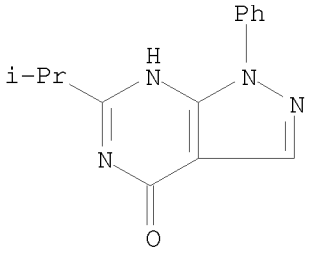
RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



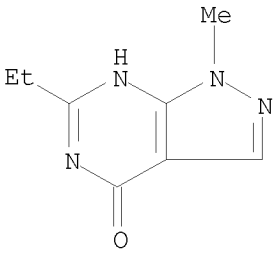
RN 130925-64-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-propyl- (CA INDEX NAME)



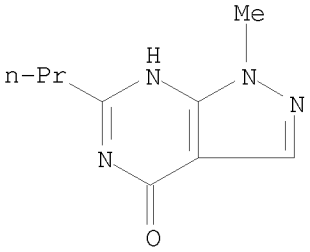
RN 130925-65-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-(1-methylethyl)-1-phenyl- (CA INDEX NAME)



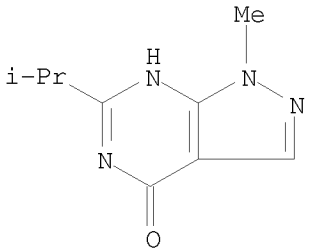
RN 130925-68-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl- (CA INDEX NAME)



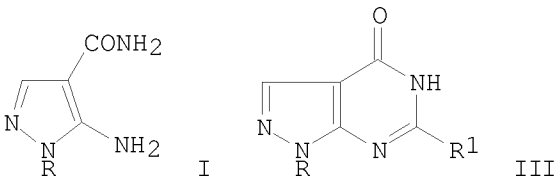
RN 130925-69-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-propyl- (CA INDEX NAME)



RN 130925-70-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(1-methylethyl)- (CA INDEX NAME)



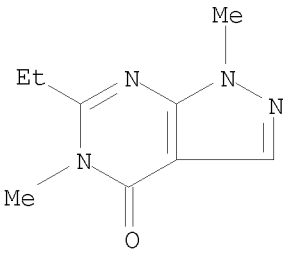
GI



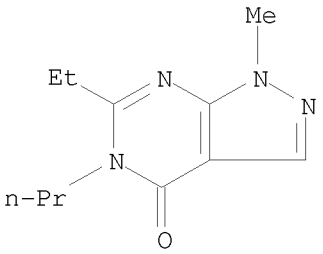
AB Reaction of 5-amino-1-phenyl-1H-pyrazole-4-carboxamide (I, R = Ph) with

R1CO2R2 (II, R1 = H, Me, Et, Pr, Me2CH, PHCH2, CO2Et, Ph; R2 = Me, Et) in the presence of EtONa-EtOH gave 1-phenylpyrazolopyrimidinones III (R = Ph). Similar treatment of I (R = Me) with II gave III (R = Me).

L4 ANSWER 29 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:34489 CAPLUS
DOCUMENT NUMBER: 100:34489
ORIGINAL REFERENCE NO.: 100:5351a,5354a
TITLE: Phosphorus pentoxide in organic synthesis. V. Phosphorus pentoxide and amine hydrochlorides as reagents in the synthesis of 1,5-dihydro-1-methyl-4H-pyrazolo[3,4-d]pyrimidin-4-ones
AUTHOR(S): Finlander, Peter; Nielsen, Soeren V.; Pedersen, Erik B.
CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.
SOURCE: Chemica Scripta (1983), 22(4), 171-6
CODEN: CSRPB9; ISSN: 0004-2056
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:34489
IT 88320-62-1P 88320-63-2P 88320-64-3P
88320-65-4P 88320-66-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antitumor activity of)
RN 88320-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1,5-dimethyl- (CA INDEX NAME)

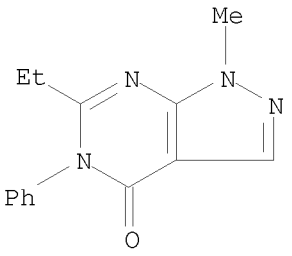


RN 88320-63-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl-5-propyl- (CA INDEX NAME)

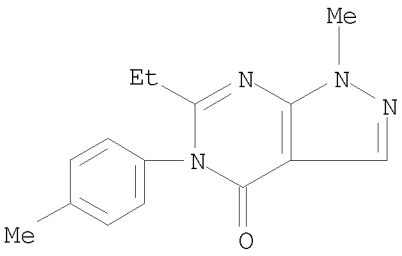


RN 88320-64-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-methyl-5-phenyl-

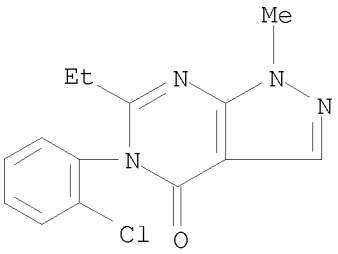
(CA INDEX NAME)



RN 88320-65-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-ethyl-1,5-dihydro-1-methyl-5-(4-methylphenyl)- (CA INDEX NAME)



RN 88320-66-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-(2-chlorophenyl)-6-ethyl-1,5-dihydro-1-methyl- (CA INDEX NAME)



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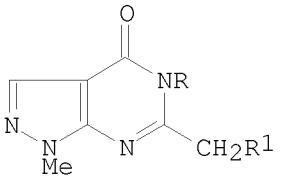
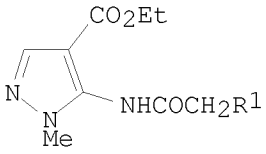
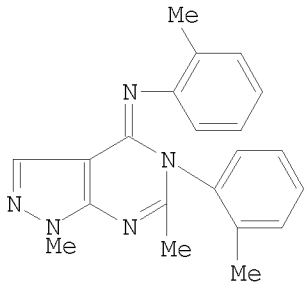


I



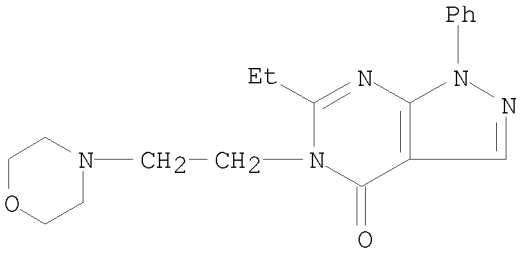
II



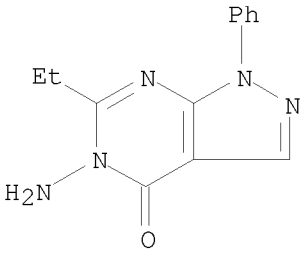
III

AB Pyrazolo[3,4-d]pyrimidinones I (R = H, alkyl, allyl, CH2Ph, Ph, substituted Ph; R1 = H, Me) were prepared by heating pyrazolecarboxylates II with P2O5, N,N-dimethylcyclohexylamine and RNH2.HCl. When 2-MeC6H4NH2.HCl was used it was also possible to isolate III. The results from pesticide and anticancer screenings are given.

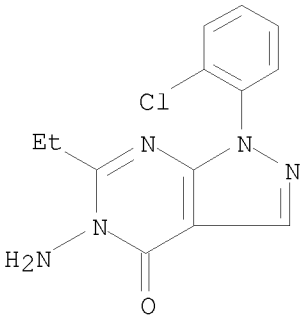
L4 ANSWER 30 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1977:567969 CAPLUS
DOCUMENT NUMBER: 87:167969
ORIGINAL REFERENCE NO.: 87:26547a,26550a
TITLE: Synthesis of condensed heterocyclic systems of pyrazole
AUTHOR(S): Alonso, G.; Madronero, R.; Nebreda, L.
CORPORATE SOURCE: Inst. Quim. Med., Madrid, Spain
SOURCE: Anales de Quimica (1968-1979) (1976), 72(11-12), 897-901
CODEN: ANQUBU; ISSN: 0365-4990
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
IT 64257-08-5P 64257-09-6P 64257-10-9P
64257-17-6P 64257-19-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 64257-08-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-ethyl-1,5-dihydro-5-[2-(4-morpholinyl)ethyl]-1-phenyl- (CA INDEX NAME)



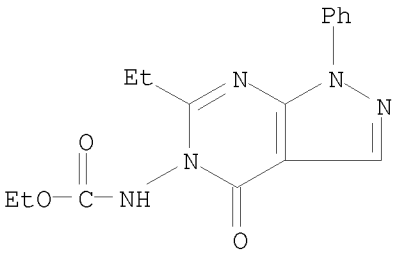
RN 64257-09-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-amino-6-ethyl-1,5-dihydro-1-phenyl-
(CA INDEX NAME)



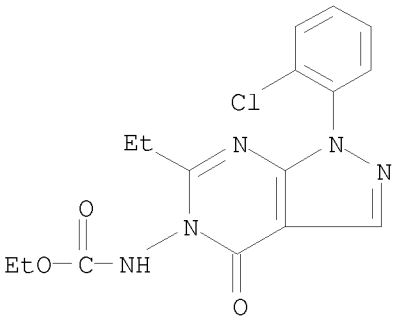
RN 64257-10-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-amino-1-(2-chlorophenyl)-6-ethyl-1,5-dihydro- (CA INDEX NAME)



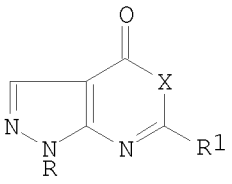
RN 64257-17-6 CAPLUS
CN Carbamic acid, (6-ethyl-1,4-dihydro-4-oxo-1-phenyl-5H-pyrazolo[3,4-d]pyrimidin-5-yl)-, ethyl ester (9CI) (CA INDEX NAME)



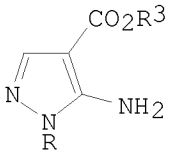
RN 64257-19-8 CAPLUS
CN Carbamic acid, [1-(2-chlorophenyl)-6-ethyl-1,4-dihydro-4-oxo-5H-pyrazolo[3,4-d]pyrimidin-5-yl]-, ethyl ester (9CI) (CA INDEX NAME)



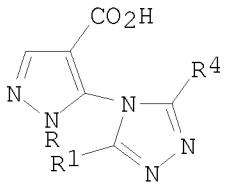
GI



I



II



III

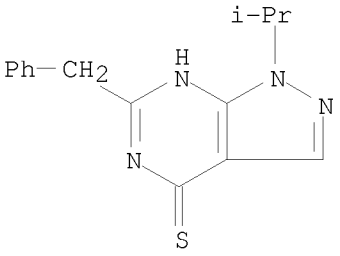
AB Pyrazolopyrimidines I (R = Ph, 2-ClC6H4; R1 = Me, Et; X = NR2, R2 = morpholinoethyl, morpholinopropyl, NH2, NHPh) were prepared by condensing EtOCH:C(CN)CO2Et with RNHNH2, hydrolyzing II (R3 = Et), cyclizing II (R3 = H) with (R1CO)2O, and treating I (X = O), with R2NH2. Reaction of I (X = O) with H2NNHCO2Et gave I (X = NNHCO2Et), whereas R4CONHNH2 (R4 = CHMe2, CH2CN, 2-furyl, 3-pyridiyl, 1-naphthyl, 2-naphthyl, 3-indolyl, 2-indolyl, Me, Ph, PhCH2) gave III and 1-naphthylacetylhydrazine gave a mixture of I (X = NNHCOCH2C10H7) and III (R4 = 1-naphthylmethyl).

L4 ANSWER 31 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:84620 CAPLUS
DOCUMENT NUMBER: 64:84620
ORIGINAL REFERENCE NO.: 64:15897g-h,15898a
TITLE: 4-Mercaptopyrazolo[3,4-d]pyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 6 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

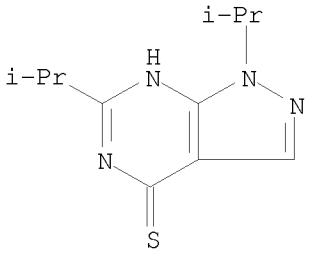
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 396924		19660131	CH 1960-1273264	19600511
PRIORITY APPLN. INFO.:			CH	19600511

IT 5494-39-3P, 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 6-benzyl-1-isopropyl- 5494-41-7P, 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 1,6-diisopropyl- 5494-44-0P, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-1-isopropyl-4-(methylthio)- 5494-45-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-(methylthio)- 5494-82-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1,6-diisopropyl- 5494-84-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-isopropyl- 5546-24-7P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]- 6109-79-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[3-(diethylamino)propyl]thio]-1,6-diisopropyl-
RL: PREP (Preparation)
(preparation of)

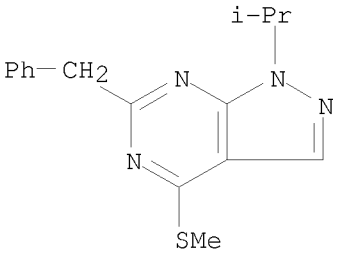
RN 5494-39-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



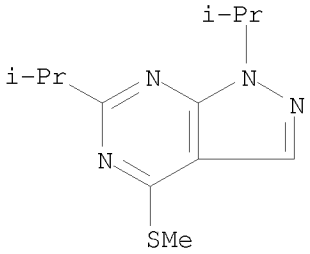
RN 5494-41-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 1,5-dihydro-1,6-bis(1-methylethyl)- (CA INDEX NAME)



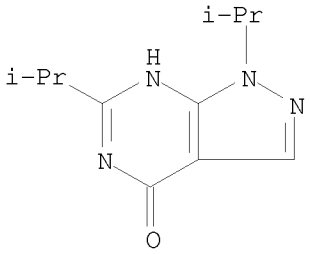
RN 5494-44-0 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(1-methylethyl)-4-(methylthio)-6-(phenylmethyl)- (CA INDEX NAME)



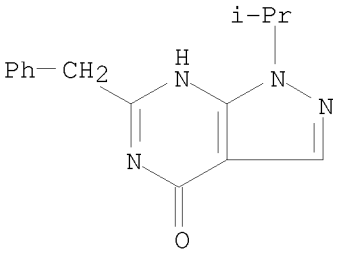
RN 5494-45-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-bis(1-methylethyl)-4-(methylthio)- (CA INDEX NAME)



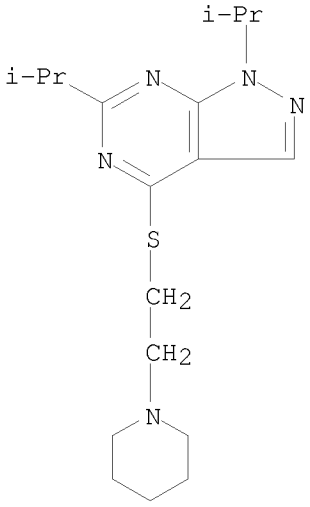
RN 5494-82-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,6-bis(1-methylethyl)- (CA INDEX NAME)



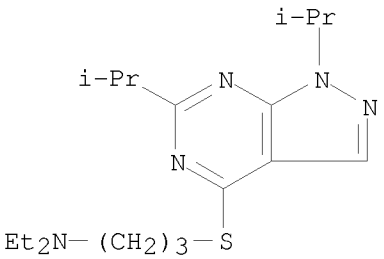
RN 5494-84-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



RN 5546-24-7 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-bis(1-methylethyl)-4-[[2-(1-piperidinyl)ethyl]thio]- (CA INDEX NAME)



RN 6109-79-1 CAPLUS
CN 1-Propanamine, 3-[[1,6-bis(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]thio]-N,N-diethyl- (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract The preparation of I from the corresponding 4-SH compds. is described. Thus, to a solution of 18.2 g. 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine, m. 195-6°, in 200 ml. pyridine is added 30 g. P2S5, the mixture refluxed 8 hrs., poured onto 3 l. ice-H2O, and kept overnight to precipitate I (R = H, R1 = Me). Similarly are prepared the SH compds. described in the preceding abstract To a solution of 20.8 g. I (R = H, R1 = Me) in 130 ml. 2N NaOH is added 24 ml. Me2SO4 and the mixture stirred at room temperature 1 hr. and kept overnight to precipitate I (R = R1 = Me), m. 66-7° (petroleum ether). Similarly are obtained the SR compds. described in the preceding abstract I possess coronary dilating properties.

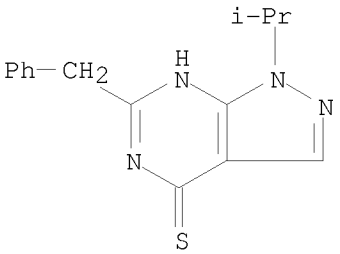
L4 ANSWER 32 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:84619 CAPLUS
DOCUMENT NUMBER: 64:84619
ORIGINAL REFERENCE NO.: 64:15897d-g
TITLE: 4-Mercaptopyrazolo[3,4-d]pyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 396923		19660131	CH 1960-1273164	19600511

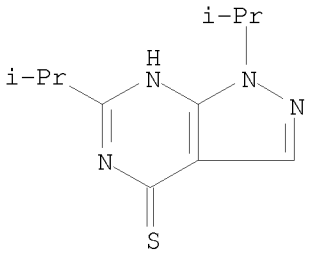
PRIORITY APPLN. INFO.: CH 19600511

IT 5494-39-3P, 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 6-benzyl-1-isopropyl- 5494-41-7P, 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 1,6-diisopropyl- 5494-43-9P, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-4-[[2-(diethylamino)ethyl]thio]-1-isopropyl-, hydrochloride 5494-44-0P, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-1-isopropyl-4-(methylthio)- 5494-45-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-(methylthio)- 5494-46-2P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[2-(diethylamino)ethyl]thio]-1,6-diisopropyl- 5494-47-3P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[2-(dimethylamino)ethyl]thio]-1,6-diisopropyl-, hydrochloride 5494-81-5P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[2-(dimethylamino)ethyl]thio]-1,6-diisopropyl- 5494-84-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-isopropyl- 5546-20-3P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]-, hydrochloride 5546-24-7P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-[(2-piperidinoethyl)thio]-6109-79-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 4-[[3-(diethylamino)propyl]thio]-1,6-diisopropyl-
RL: PREP (Preparation)
(preparation of)

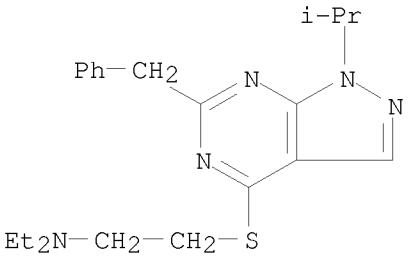
RN 5494-39-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



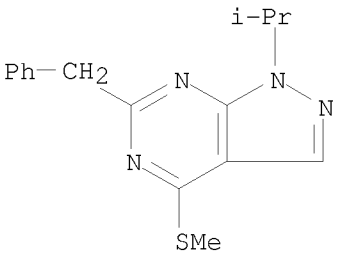
RN 5494-41-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 1,5-dihydro-1,6-bis(1-methylethyl)- (CA INDEX NAME)



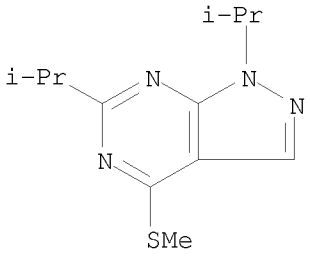
RN 5494-43-9 CAPLUS
CN Ethanamine, N,N-diethyl-2-[[1-(1-methylethyl)-6-(phenylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]thio]-, hydrochloride (1:1) (CA INDEX NAME)



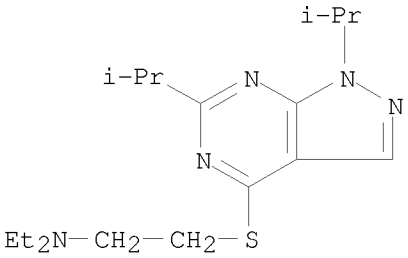
RN 5494-44-0 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(1-methylethyl)-4-(methylthio)-6-(phenylmethyl)- (CA INDEX NAME)



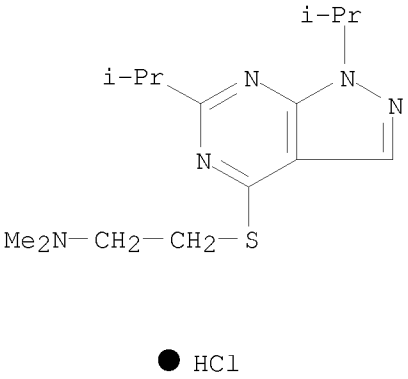
RN 5494-45-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-bis(1-methylethyl)-4-(methylthio)- (CA INDEX NAME)



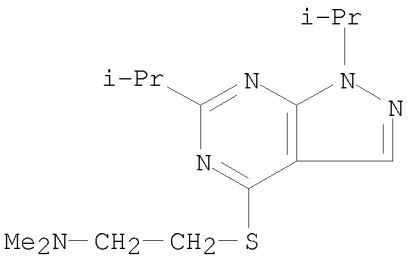
RN 5494-46-2 CAPLUS
CN Ethanamine, 2-[[1,6-bis(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]thio]-N,N-diethyl- (CA INDEX NAME)



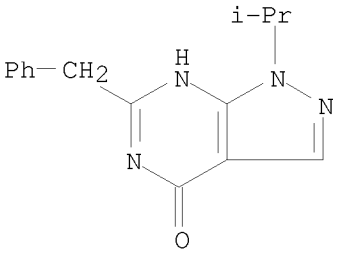
RN 5494-47-3 CAPLUS
CN Ethanamine, 2-[[1,6-bis(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]thio]-N,N-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)



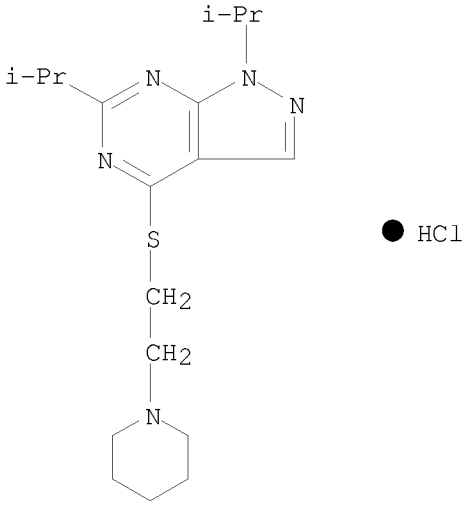
RN 5494-81-5 CAPLUS
CN Ethanamine, 2-[[1,6-bis(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]thio]-N,N-dimethyl- (CA INDEX NAME)



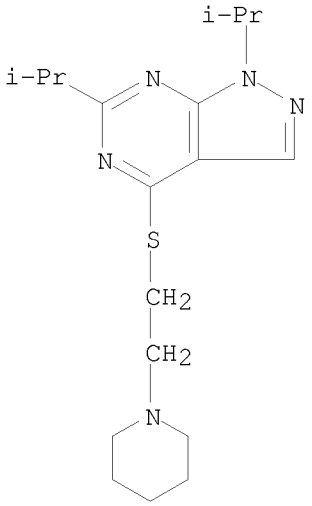
RN 5494-84-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



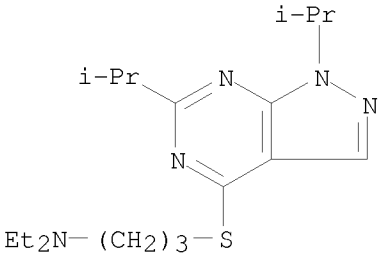
RN 5546-20-3 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-bis(1-methylethyl)-4-[[2-(1-
piperidinyl)ethyl]thio]-, hydrochloride (1:1) (CA INDEX NAME)



RN 5546-24-7 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-bis(1-methylethyl)-4-[[2-(1-
piperidinyl)ethyl]thio]- (CA INDEX NAME)



RN 6109-79-1 CAPLUS
CN 1-Propanamine, 3-[[1,6-bis(1-methylethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-yl]thio]-N,N-diethyl- (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

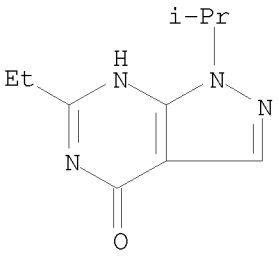
AB cf. following abstract The title compds. (I) are prepared by treating the corresponding 4-halo compds. with thiourea, metal salts of H2S, lower-alkyl, amino- or ammonium-lower alkyl mercaptans. Thus, a stirred mixture of 50 ml. PhCH2CN, 2.3 g. Na (small pieces), and 9.9 g. 2-isopropyl-3-amino-4-carbethoxypyrazole is heated at 110-20° 4 hrs., cooled, 100 ml. alc. added, the mixture taken to dryness in vacuo, the residue taken up in 150 ml. 2N NaOH, and the alkaline solution washed with CHCl3 and acidified to pH 5-6 with 6N HCl to precipitate 1-isopropyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (II), m. 165-6° (alc.). A mixture of 10 g. II and 100 ml. POCl3 is heated at 110° 5 hrs. and evaporated to dryness in vacuo, the residue taken up in H2O and extracted with CHCl3, the extract washed with N NaOH, dried over Na2SO4, and the CHCl3 evaporated in vacuo to yield the 4-Cl (III) analog of II. A solution of III and 8.5 g. thiourea in 150 ml. alc. is refluxed 12 hrs., concentrated to 60 ml., and cooled to afford I (R = H, R1 = PhCH2, m. 145-7°. Similarly are prepared the following I (R, R1, b.p. (mm.), and m.p. given): H, Me, --, 226-8°; H, CHMe2, --, 170-1°;

Me, Me, --, 66-7°; (CH2)2NEt2, PhCH2, --, --(hydrochloride m. 160°); Me, PhCH2, --, 84-5°; Me, CHMe2, 106-9° (0.05), --; (CH2)2NEt2, CHMe2, 138-40° (0.05), --; (CH2)3NEt2, CHMe2, 149-51° (0.02), --; 2-(piperidine)ethyl, CHMe2, --, -- (hydrochloride m. 163-5°); (CH2)2NMe2, CHMe2, --, -- (hydrochloride m. 178-80°).

L4 ANSWER 33 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:84617 CAPLUS
DOCUMENT NUMBER: 64:84617
ORIGINAL REFERENCE NO.: 64:15896h,15897a-b
TITLE: Novel pyrazolopyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

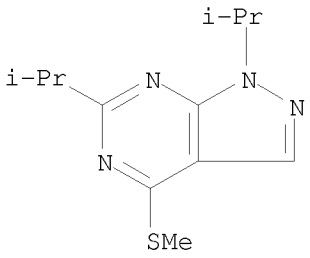
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 396927		19660113	CH 1960-509965	19600511

PRIORITY APPLN. INFO.: CH 19600511
IT 5543-55-5P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-ethyl-1-isopropyl-
RL: PREP (Preparation)
(preparation of)
RN 5543-55-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-(1-methylethyl)-
(CA INDEX NAME)



AB The title compds. are prepared by cyclization of substituted pyrroles. Thus, a mixture of 30 g. 2-isopropyl-3-amino-4-cyanopyrazole (I) and 68 ml. Ac2O is refluxed 10 hrs., the mixture evaporated to dryness, the residue recrystd. from Et2O and subsequently from H2O, and the mother liquor concentrated to give a viscous mass (II) containing the acetylamino derivative of I. A mixture of II (3.84 g.), 14 ml. 10% aqueous KOH, and 30 ml. 3% H2O2 is heated on a steam bath 0.5 hr., filtered, and the filtrate acidified with 2N HCl to give 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine (III), m. 195-6° (alc.). Similarly prepared is the 6-Et derivative of III, m. 180-2° (EtOH). The compds. possess coronary dilating properties.

L4 ANSWER 34 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:79294 CAPLUS
DOCUMENT NUMBER: 64:79294
ORIGINAL REFERENCE NO.: 64:14897f-g
TITLE: Relation between synergism and metabolism of dimethoate in mammals and insects
AUTHOR(S): Uchida, T.; Zschintzsch, J.; O'Brien, R. D.
CORPORATE SOURCE: Cornell Univ., Ithaca, NY, USA
SOURCE: Toxicology and Applied Pharmacology (1966), 8(2), 259-265
CODEN: TXAPA9; ISSN: 0041-008X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 5494-45-1P, 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-diisopropyl-4-(methylthio)-
RL: PREP (Preparation)
(preparation of)
RN 5494-45-1 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1,6-bis(1-methylethyl)-4-(methylthio)- (CA INDEX NAME)

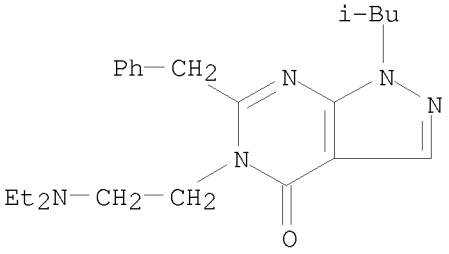


AB Toxicol. Appl. Pharmacol. 8(2), 259-65(1966)(Eng). EPN (Et p-nitrophenyl thiono-benzenephosphate) synergizes the toxicity of dimethoate profoundly in female mice, mildly in female guinea pigs, and not at all in female houseflies (Wilson and G strains) or milkweed bugs. These findings parallel the observations that EPN blocks di-methoate metabolism profoundly (80%) in mice, less in guinea pigs (60%), and not at all in houseflies and milkweed bugs. Synergism in this pair of compds. is caused by blockade of metabolism. However, the ability of EPN to distinguish between the amidase and phosphatase pathways is not so clear-cut as in the corresponding carboxyesterase and phosphatase pathways for malathion, whose toxicity is also synergized by EPN.

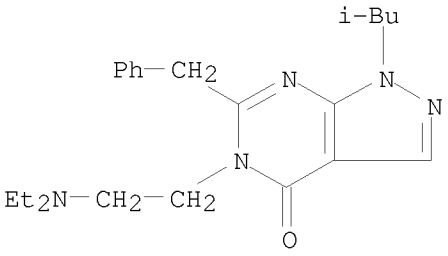
L4 ANSWER 35 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:22610 CAPLUS
DOCUMENT NUMBER: 62:22610
ORIGINAL REFERENCE NO.: 62:4037e-h
TITLE: 4-Carboxyalkylthio-5-aryl pyrimidines
PATENT ASSIGNEE(S): Spofa Sdruzeni Podniku pro Zdravotnickou Vyrobu
SOURCE: 6 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6400014		19640706	NL 1964-14	19640103
BE 642046			BE	
FR 1381675			FR	
GB 1046258			GB	
PRIORITY APPLN. INFO.:			CS	19630103

IT 95225-07-3 100321-66-2
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 95225-07-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)-
(CA INDEX NAME)



RN 100321-66-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)-
, hydrochloride (1:?) (CA INDEX NAME)



●x HCl

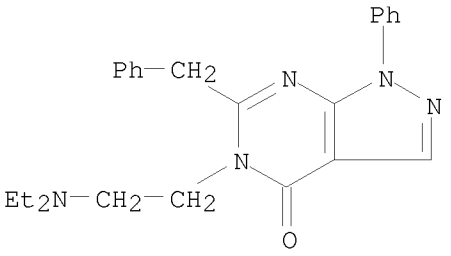
GI For diagram(s), see printed CA Issue.

AB The title compds. (I) were prepared by the sulfuration of II with P2S5 in non-aqueous inert organic solvents at 80-200°, and addition of haloalkyl carboxylic acids to III in aqueous or aqueous alc. metal hydroxide solution Thus,
17.2 g. II (R = X = H) and 50 g. P2S5 was refluxed 2 hrs. in 200 ml. anhydrous C5H5N, the C5H5N distilled in vacuo, and the residue treated with H2O to give 8.0 g. III (R = X = H), m. 168-9° (sublimation) (H2O), of which 5.65 g. was dissolved in a solution of 1.32 g. NaOH in 60 ml. 65% aqueous EtOH, the solution cooled to -5°, 4.05 g. ClCH2CO2Et added dropwise (an oil separated), the mixture is concentrated to 1/3 volume, 40 ml. 10% NaOH added,
the mixture stirred 8 hrs. at 40-50° and charcoaled, and the pH adjusted to 4-5 to give 4.7 g. I (R = X = R1 = H, n = O), m. 203-5° (decomposition) (40% EtOH). III (R = H, X = 4-Cl), m. 245° (5.91 g.), obtained from II (R = H, X = 4-Cl,) and 6.1 g. ω-bromovalerate was refluxed 2 hrs. in a solution of 1.17 g. NaOH, 40 ml. EtOH, and 20 ml. H2O. The ester obtained was hydrolyzed with 3.5 g. NaOH in 20 ml. H2O; acidification with AcOH gave 3.5 g. I (R = R1 = H, X = 4-Cl, n = 3), m. 126° (30% EtOH). In the same way, III (R = H, X = 2-Cl), m. 246° (decomposition), and I (R = H, X = 2-Cl, R1 = Me, n = 0), m. 183°; and III (R = Me, X = H), m. 180°, and I (R = Me, X = R1 = H, n = 3), m. 109-10°, were obtained. I were useful against virus infections.

L4 ANSWER 36 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:22609 CAPLUS
DOCUMENT NUMBER: 62:22609
ORIGINAL REFERENCE NO.: 62:4037c-e
TITLE: Pyrazolo[3,4-d]pyrimidines
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

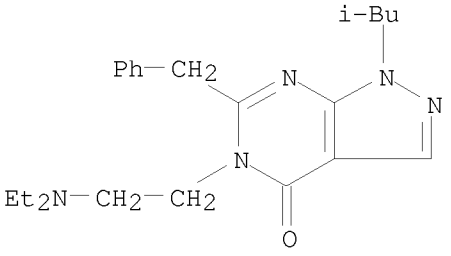
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 973361		19641028	GB 1961-17103	19610510
PRIORITY APPLN. INFO.:			CH	19600511

IT 1177-04-4 95225-07-3 100321-66-2
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 1177-04-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-,
hydrochloride (1:1) (CA INDEX NAME)



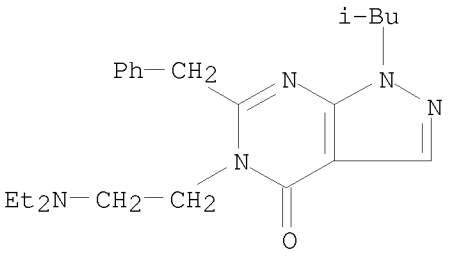
● HCl

RN 95225-07-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)-
(CA INDEX NAME)



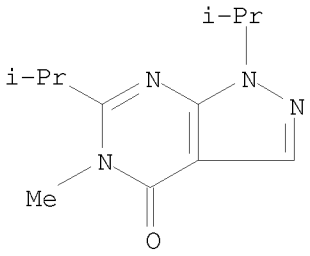
RN 100321-66-2 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)-
, hydrochloride (1:?) (CA INDEX NAME)

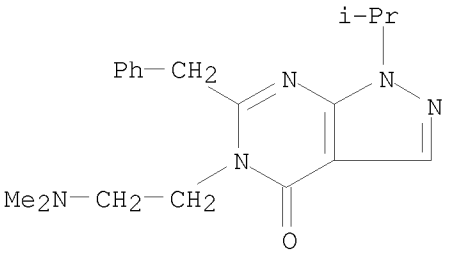


●x HCl

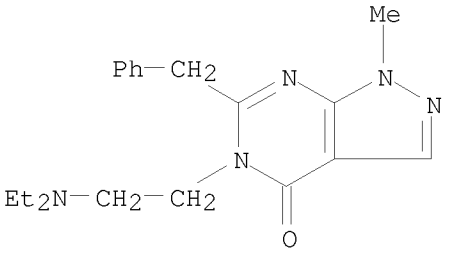
IT 1143-77-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1,6-diisopropyl-5-methyl- 1168-08-7P,
4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-isopropyl-
1168-43-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-
1168-44-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-, hydrochloride
1173-78-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-1-sec-butyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-, hydrochloride
1173-93-9P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[3-(diethylamino)propyl]-1,5-dihydro-1-isopropyl-
1173-94-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[3-(diethylamino)propyl]-1,5-dihydro-1-isopropyl-,
hydrochloride 1180-45-6P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-6-(diphenylmethyl)-1,5-dihydro-1-isopropyl-
1229-51-2P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-1,5-dihydro-1-isopropyl-5-methyl- 1237-01-0P,
4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1,6-diisopropyl- 1242-91-7P
, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-isopropyl-,
hydrochloride 1248-40-4P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-isopropyl-
1248-41-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-isopropyl-, hydrochloride
1254-49-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-
1447-19-4P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-1-sec-butyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-
101405-08-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 1143-77-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-5-methyl-1,6-bis(1-methylethyl)- (CA INDEX NAME)



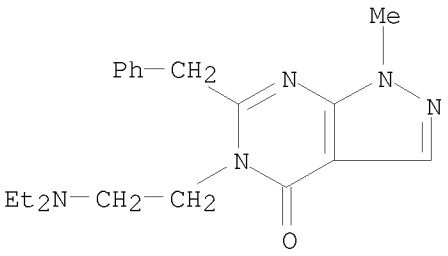
RN 1168-08-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-
(CA INDEX NAME)



RN 1168-43-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-6-(phenylmethyl)- (CA
INDEX NAME)

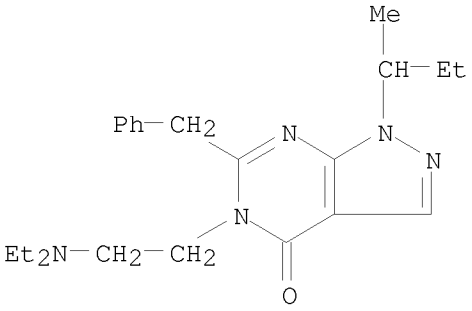


RN 1168-44-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-6-(phenylmethyl)-,
hydrochloride (1:1) (CA INDEX NAME)



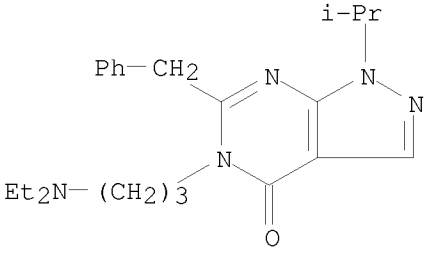
● HCl

RN 1173-78-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(1-methylpropyl)-6-(phenylmethyl)-
, hydrochloride (1:1) (CA INDEX NAME)



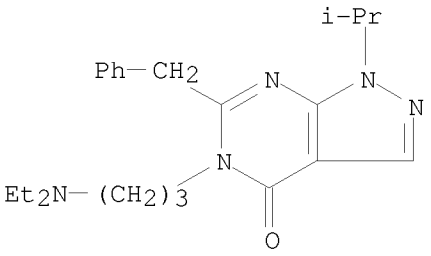
● HCl

RN 1173-93-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[3-(diethylamino)propyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-
(CA INDEX NAME)



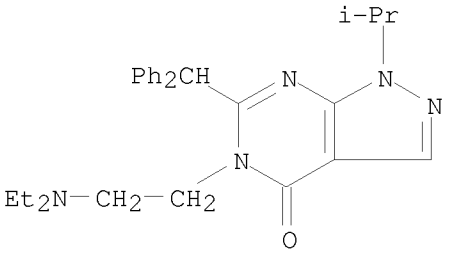
RN 1173-94-0 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[3-(diethylamino)propyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-
, hydrochloride (1:1) (CA INDEX NAME)

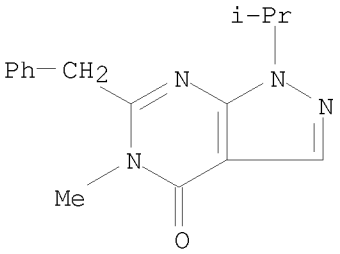


● HCl

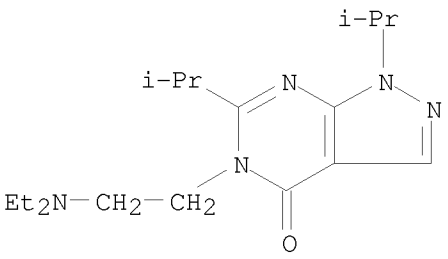
RN 1180-45-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-6-(diphenylmethyl)-1,5-dihydro-1-(1-methylethyl)-
(CA INDEX NAME)



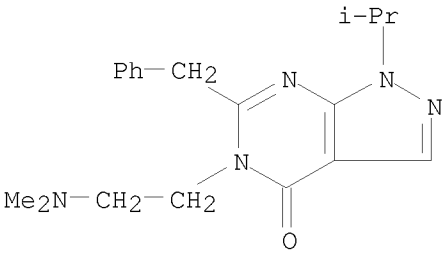
RN 1229-51-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-5-methyl-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



RN 1237-01-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1,6-bis(1-methylethyl)- (CA INDEX
NAME)

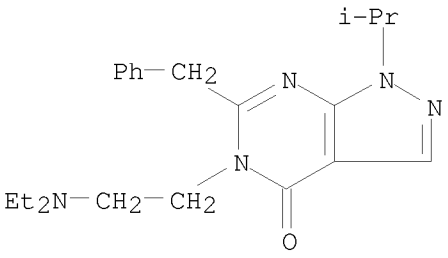


RN 1242-91-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-
, hydrochloride (1:1) (CA INDEX NAME)

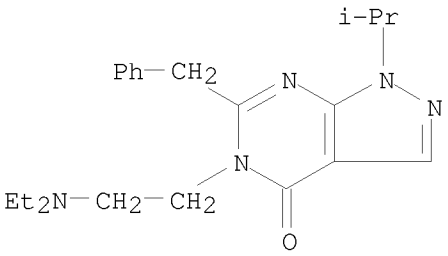


● HCl

RN 1248-40-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-
(CA INDEX NAME)

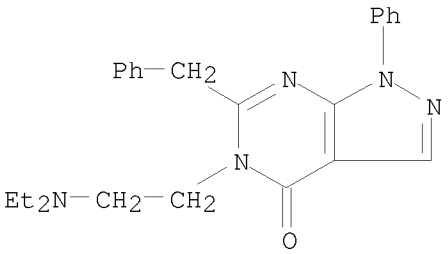


RN 1248-41-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-,
hydrochloride (1:1) (CA INDEX NAME)

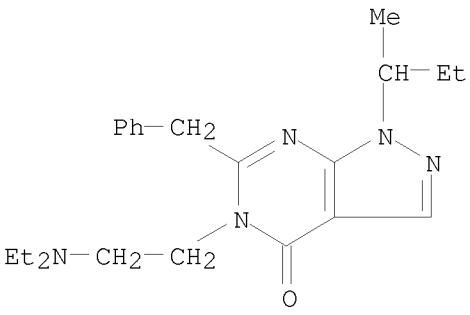


● HCl

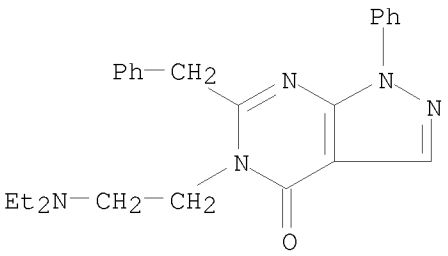
RN 1254-49-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)

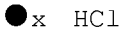


RN 1447-19-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(1-methylpropyl)-6-(phenylmethyl)-
(CA INDEX NAME)



RN 101405-08-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-,
hydrochloride (1:?) (CA INDEX NAME)





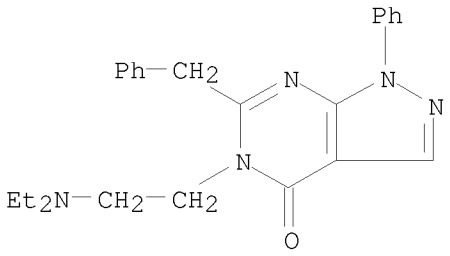
GI For diagram(s), see printed CA Issue.

AB The title compds. (I) were prepared by alkylating a 1,6-disubstituted 4-hydroxypyrazolo[3,4-d]pyrimidine with a dialkylaminoalkyl chloride or Me2SO4. Thus, a solution of 1.15 g. Na in 40 ml. EtOH was added to 14.1 g. 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine followed by 7.5 g. Et2NCH2CH2Cl and the mixture refluxed 4 hrs. to give the hydrochloride of I (R1 = sec-Bu, R2 = Et2NCH2CH2, R3 = PhCH2), m. 147-8°. The following I were prepared similarly (R1, R2, R3, m.p. free base, and m.p. hydrochloride given): iso-Pr, Me, PhCH2, 96-7°, --; iso-Pr, Me2NCH2CH2, PhCH2, 115-17°, 229-31°; iso-Pr, Et2NCH2CH2, PhCH2, --, 202-3°; iso-Pr, Et2N(CH2)3, PhCH2, 70-1°, 173-5°; Me, Et2NCH2CH2, PhCH2, 83-5°, 219°; Ph, Et2NCH2CH2, PhCH2, 103-5°, 225°; iso-Pr, Et2NCH2CH2, Me, --, --; iso-Pr, Me, iso-Pr, 75-7°, --; iso-Pr, Et2NCH2CH2, iso-Pr, --(b0.05 138-40°), --; iso-Pr, Et2NCH2CH2, Ph2CH, 124-5°, --. The title compds. had coronary dilating properties.

L4 ANSWER 37 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:22608 CAPLUS
DOCUMENT NUMBER: 62:22608
ORIGINAL REFERENCE NO.: 62:4037a-c
TITLE: O-(α-Tetrahydropyranyl)-S-alkoxycarbonyl thiamines with vitamin B1 activity
INVENTOR(S): Takamizawa, Akira; Hirai, Kentaro
PATENT ASSIGNEE(S): Shionogi & Co., Ltd.
SOURCE: 17 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR M2755		19640928	FR	
DE 1226586			DE	
PRIORITY APPLN. INFO.:			JP	19620727

OTHER SOURCE(S): MARPAT 62:22608
IT 1177-04-4
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 1177-04-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-, hydrochloride (1:1) (CA INDEX NAME)



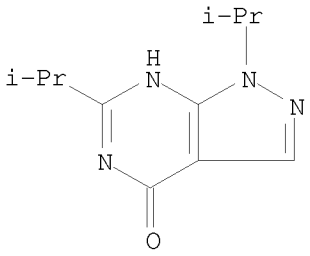
GI For diagram(s), see printed CA Issue.
AB I (R = 2-pyranyl) have a rapid and long-lasting vitamin B1 activity. They are prepared by the reaction of I (R = H, II) with 4H-dihydropyran in the presence of an acid catalyst. II are prepared from the alkali salts III (where M = Na or K) of the thiol form of thiamine (IV) with compds. XCOYR, where X is a halogen atom. Thus, 0.35 mL. HCl is added to a suspension of 1 g. S-ethoxycarbonylthiamine (V) in 10 mt. 4H-dihydropyran, the mixture stirred, the separated crystals are taken up in H2O, the solution is shaken with Et2O, and NH4OH added to precipitate 0.80 g. O-(α-tetrahydropyranyl)-S-(ethoxycarbonyl)thiamine, m. 73-4° (H2O + EtOH). For the preparation of V, m. 140° (decomposition) (AcOEt), IV.HCl is dissolved in aqueous NaOH, the solution saturated with NaCl, and ClCO2Et

added. Other compds. prepared are O-(α-tetrahydropyranyl)-S-(butoxycarbonyl)thiamine, m. 125°; S-butoxycarbonylthiamine, m. 139-40° (decomposition); O-(α-tetrahydropyranyl)-S-ethylthiocarbonylthiamine, m. 102-3°; and S-ethylthiocarbonylthiamine, m. 136-7° (decomposition).

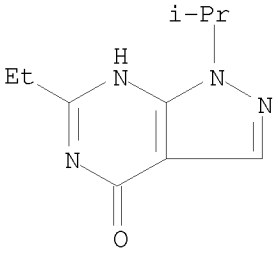
L4 ANSWER 38 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:68272 CAPLUS
DOCUMENT NUMBER: 60:68272
ORIGINAL REFERENCE NO.: 60:12027a-c
TITLE: 1-Isopropyl-4-hydroxypyrazolo[3,4-d]pyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1156415		19631031	DE	
CH 396926			CH	
PRIORITY APPLN. INFO.:			CH	19600511

IT 5494-82-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1,6-diisopropyl-
5543-55-5P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-ethyl-1-isopropyl-
88618-14-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-isobutyl-1-isopropyl-
RL: PREP (Preparation)
(preparation of)
RN 5494-82-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,6-bis(1-methylethyl)-
(CA INDEX NAME)

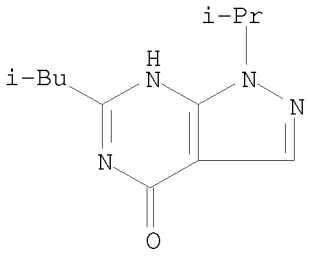


RN 5543-55-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-(1-methylethyl)-
(CA INDEX NAME)



RN 88618-14-8 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-methylethyl)-6-(2-methylpropyl)- (CA INDEX NAME)



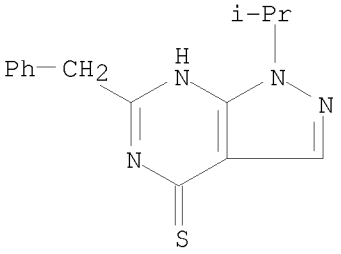
GI For diagram(s), see printed CA Issue.

AB 2-Isopropyl-3-amino-4-carbethoxypyrazole (39.6 g.) in 160 cc. isobutyronitrile and 9.2 g. Na was heated slowly over 1 hr. to 110°, and the mixture kept 4 hrs. at 110° to give 16 g. I (R = iso-Pr), m. 175-7°. Similarly prepared were the following I (R and m.p. given): Me, 195-6°; Me2CHCH2, 114-16°; Et, 180-2°. I are coronary dilators.

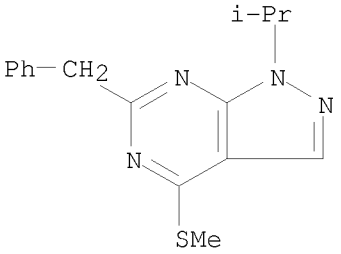
L4 ANSWER 39 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:60960 CAPLUS
DOCUMENT NUMBER: 60:60960
ORIGINAL REFERENCE NO.: 60:10698a-c
TITLE: 1-Alkyl-6-aralkylpyrazolo[3,4-d]pyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1161281		19640116	DE 1961-C23979	19610426
GB 937726			GB	
PRIORITY APPLN. INFO.:			CH	19600511

IT 5494-39-3P, 1H-Pyrazolo[3,4-d]pyrimidine-4-thiol, 6-benzyl-1-isopropyl- 5494-44-0P, 1H-Pyrazolo[3,4-d]pyrimidine, 6-benzyl-1-isopropyl-4-(methylthio)- 5494-84-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-isopropyl-
RL: PREP (Preparation)
(preparation of)
RN 5494-39-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidine-4-thione, 1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)

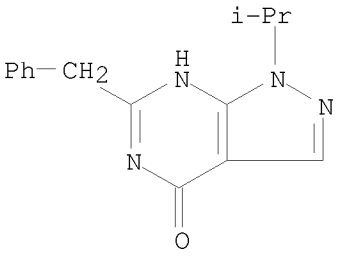


RN 5494-44-0 CAPLUS
CN 1H-Pyrazolo[3,4-d]pyrimidine, 1-(1-methylethyl)-4-(methylthio)-6-(phenylmethyl)- (CA INDEX NAME)



RN 5494-84-8 CAPLUS

CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)

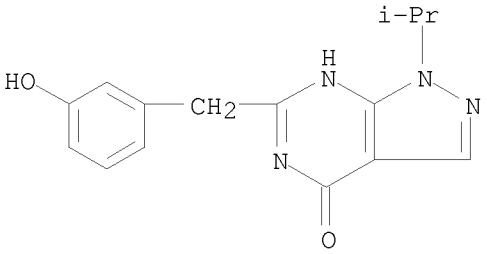


AB To 13 g. 1-isopropyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (I), m. 165-6° (from PhCH2CN, Na, and 2-isopropyl-3-amino-4-carbethoxypyrazole), in 100 cc. C5H5N was added 15 g. P2S5, the whole refluxed 8 hrs., and the mixture poured on ice-H2O to give 8 g. yellow 4-SH analog (II) of I, m. 145-7° (EtOH). II (14 g.) in 60 cc. 2N NaOH treated with 13 g. Me2SO4, and the mixture stirred 2 hrs. gave 12.7 g. 4-SMe analog of I, m. 84-5° (petr. ether). The compds. showed coronary dilatory effects.

L4 ANSWER 40 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:16883 CAPLUS
DOCUMENT NUMBER: 60:16883
ORIGINAL REFERENCE NO.: 60:2981a-e
TITLE: 4-Hydroxypyrazolo[3,4-d]pyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 10 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1153023		19630822	DE	
CH 396925			CH	
GB 937724			GB	
PRIORITY APPLN. INFO.:			CH	19600511

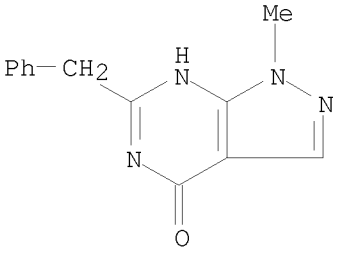
IT 1082647-92-4P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(4-Hydroxypyrazolo[3,4-d]pyrimidines)
RN 1082647-92-4 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[(3-hydroxyphenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)



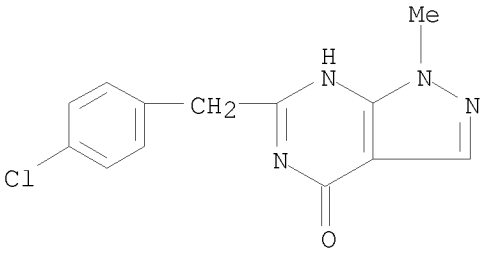
IT 91803-32-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-methyl-
92023-17-1P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-(p-chlorobenzyl)-1-methyl- 92193-40-3P,
1H-Pyrazolo[3,4-d]pyrimidine-1-ethanol, 6-benzyl-4-hydroxy-
92553-22-5P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-(p-chlorobenzyl)-1-isopropyl- 93022-43-6P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-sec-butyl-
93022-45-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
1-isopropyl-6-phenethyl- 93022-51-6P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1-isopropyl-6-(o-methoxybenzyl)-
93022-79-8P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
1-methyl-6-(3,4,5-trimethoxybenzyl)- 93726-15-9P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-(1,2-dimethylpropyl)-
93726-16-0P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-benzyl-1-(1-ethylpropyl)- 93726-17-1P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-(α-ethylbenzyl)-1-isopropyl-
93726-25-1P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-(p-ethoxybenzyl)-1-isopropyl- 94000-61-0P,

1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1-isopropyl-6-salicyl-
94263-95-3P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
1-isopropyl-6-(3,4,5-trimethoxybenzyl)- 94707-90-1P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1-isopropyl-6-(m-methoxybenzyl)-
94804-42-9P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
1-isopropyl-6-(3-methoxy-2-methylbenzyl)- 95158-25-1P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-(3-ethoxy-1-methylpropyl)-
95168-04-0P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-(2,3-dimethoxybenzyl)-1-methyl- 96001-11-5P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-(diphenylmethyl)-1-isopropyl-
RL: PREP (Preparation)
(preparation of)

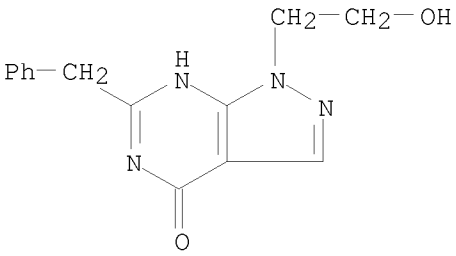
RN 91803-32-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(phenylmethyl)-
(CA INDEX NAME)



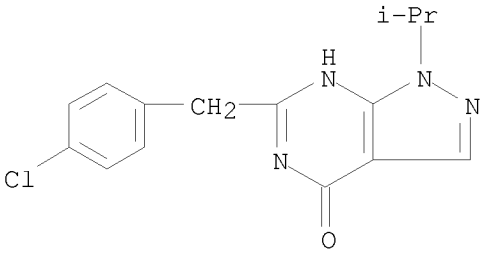
RN 92023-17-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-chlorophenyl)methyl]-1,5-dihydro-1-methyl- (CA INDEX NAME)



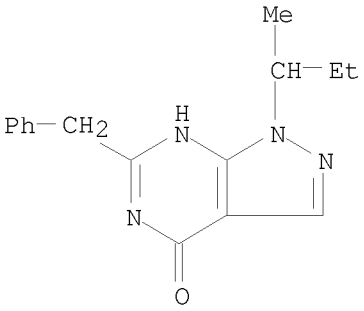
RN 92193-40-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-hydroxyethyl)-6-(phenylmethyl)- (CA INDEX NAME)



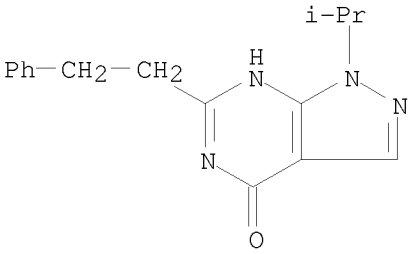
RN 92553-22-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-chlorophenyl)methyl]-1,5-dihydro-1-(1-methylethyl)- (CA INDEX NAME)



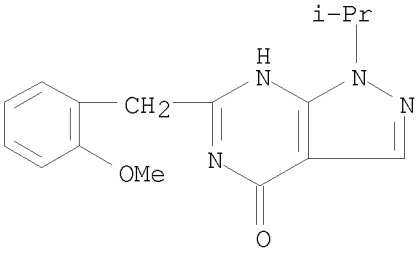
RN 93022-43-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylpropyl)-6-(phenylmethyl)- (CA INDEX NAME)



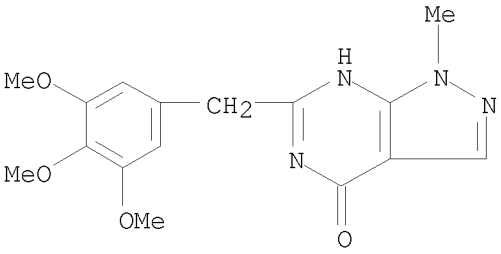
RN 93022-45-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylethyl)-6-(2-phenylethyl)- (CA INDEX NAME)



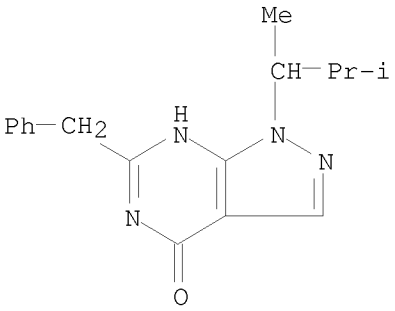
RN 93022-51-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-6-[(2-methoxyphenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)



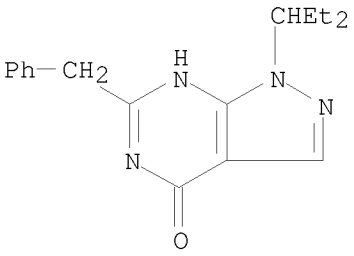
RN 93022-79-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-methyl-6-[(3,4,5-trimethoxyphenyl)methyl]- (CA INDEX NAME)



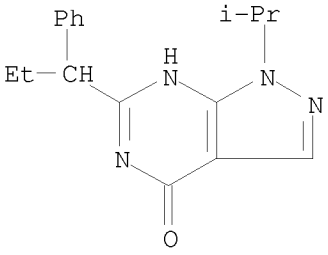
RN 93726-15-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(1,2-dimethylpropyl)-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)



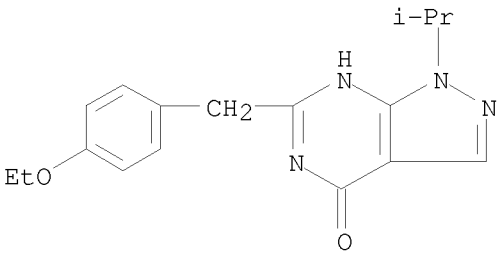
RN 93726-16-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1-(1-ethylpropyl)-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)



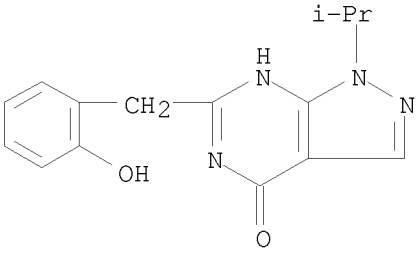
RN 93726-17-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylethyl)-6-(1-phenylpropyl)- (CA INDEX NAME)



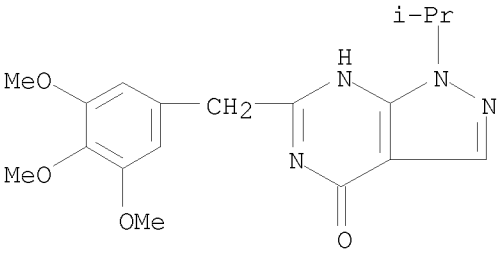
RN 93726-25-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-ethoxyphenyl)methyl]-1,5-dihydro-1-(1-methylethyl)- (CA INDEX NAME)



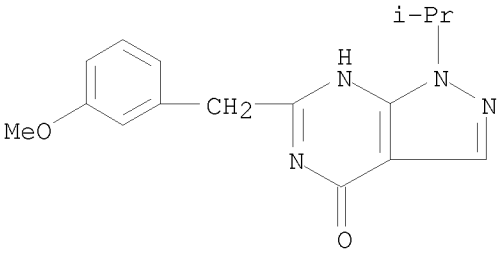
RN 94000-61-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(2-hydroxyphenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)



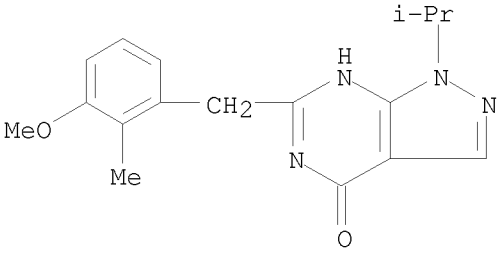
RN 94263-95-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-methylethyl)-6-[(3,4,5-trimethoxyphenyl)methyl]- (CA INDEX NAME)



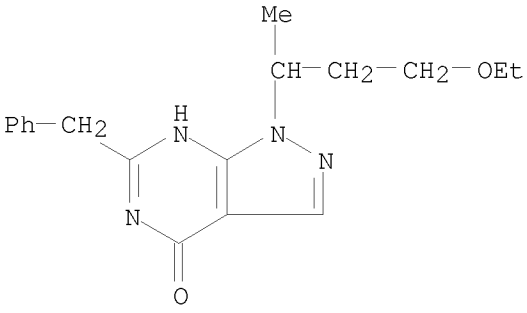
RN 94707-90-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(3-methoxyphenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)



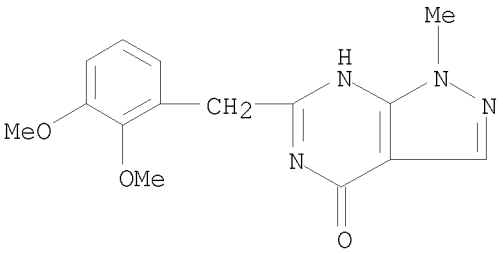
RN 94804-42-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-6-[(3-methoxy-2-methylphenyl)methyl]-1-(1-methylethyl)- (CA INDEX NAME)



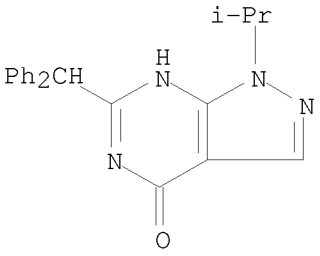
RN 95158-25-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(3-ethoxy-1-methylpropyl)-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)



RN 95168-04-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-[(2,3-dimethoxyphenyl)methyl]-1,5-dihydro-1-methyl- (CA INDEX NAME)



RN 96001-11-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(diphenylmethyl)-1,5-dihydro-1-(1-methylethyl)- (CA INDEX NAME)



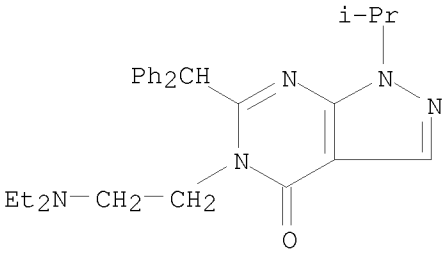
GI For diagram(s), see printed CA Issue.
AB 1-R1, 3-R2, 6-R3-substituted 4-hydroxy pyrazolo[3,4-d]pyrimidines (R1 = H, alkyl, hydroxyalkyl, or oxaalkyl; R2 = H or low-mol.-weight alkyl; R3 = eventually substituted phenylalkyl or diphenylalkyl radicals) are prepared Thus, 19.7 g. 2-isopropyl-3-amino-4-carbethoxypyrazole and 45 g. β-phenylpropionitrile in 30 cc. absolute PhMe are added to 4.6 g. powdered Na in 85 cc. absolute PhMe at 90-5° with stirring, the mixture stirred 5 hrs. at 90-5°, 50 cc. alc. added, the solution evaporated to dryness, the residue extracted with N NaOH and PhMe, and the alkaline solution neutralized with 6N
HCl to precipitate 8.7 g. 1-isopropyl-4-hydroxy-(6-R-substituted)-pyrazolo[3,4-d]pyrimidine(I) (R = β-phenylethyl), m. 124-5° (alc.).
Similarly prepared are the following I (R and m.p. given): m-hydroxybenzyl, 226-7° (alc.); p-chlorobenzyl (II), 181-2° (alc.); 3,4,5-trimethoxy-phenylmethyl, 195-6° (alc.); p-ethoxybenzyl, 175-6° (alc.); m-methoxybenzyl, 155-8° (alc.); o-methoxybenzyl, 157-9° (EtOH); 2-methyl-3-methoxybenzyl, 150-1° (EtOH); diphenylmethyl, 226-7° (EtOH); α-phenylpropyl, 142-3°(alc.). Also prepared are the following 1-methyl-4-hydroxy-(6-R-substituted)-pyrazolo[3,4-d]pyrimidines (R and m.p. given): benzyl, 236-7° (EtOH); 3,4,5-trimethoxyphenylmethyl, 245° (CHCl3-petr. ether); p-chlorobenzyl, 268-70° (HCONMe2-H2O); 2,3-dimethoxyphenylmethyl, 190-1° (alc.). The following (1-R-substituted)-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidines are prepared (R and m.p. given): sec-butyl, 154-5°(alc.); pent-3-yl, 144-5° (absolute alc.); β-hydroxyethyl, 194-5°(alc.); 1-ethoxybut-3-yl, 111-12° (MeOH-H2O); H, 290-2° (EtOH); 3-methylbut-2-yl, 157-8° (EtOH). Also prepared are these starting materials: 2-(β-hydroxyethyl)-3-amino-4-carbethoxypyrazole, b0.6

180°, m. 89-91°; 2-[1-ethoxybut-3-yl]-3-amino-4-carbethoxypyrazole, b0.1 120-5°; 2-isopropyl-3-[α-ethoxy-β-(p-chlorophenyl)ethylidenamino]pyrazole-4-carboxamide; 2-isopropyl-3-(p-chlorophenylacetamido)-4-carboxypyrazole; 1-isopropyl-4-oxo-6-(p-chlorobenzyl)pyrazolo[3,4-d]oxazine; 2-isopropyl-3-(p-chlorophenylacetamido)-4-pyrazolecarbonitrile.

L4 ANSWER 41 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:469190 CAPLUS
DOCUMENT NUMBER: 59:69190
ORIGINAL REFERENCE NO.: 59:12821a-e
TITLE: Pyrazine derivatives
INVENTOR(S): Camerino, Bruno; Palamidessi, Giorgio
PATENT ASSIGNEE(S): Societa Farmaceutici Italia
SOURCE: 9 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 928151		19630606	GB 1959-24146	19590714
DE 1204233			DE	
DE 1226104			DE	
US 3098069		19630716	US 1962-222949	19620911

PRIORITY APPLN. INFO.: GB 19590714
IT 1180-45-6
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 1180-45-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-6-(diphenylmethyl)-1,5-dihydro-1-(1-methylethyl)-
(CA INDEX NAME)



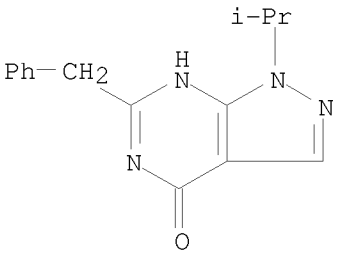
GI For diagram(s), see printed CA Issue.
AB 3- and 3,5-Substituted 2-aminopyrazines (I) were prepared These products have bactericidal activity. 2-Aminopyrazine (95.11 g.) and 326.5 g. NaOAc.3H2O in 1480 ml. AcOH treated in 2-3 hrs. in the dark with 112.7 ml. Br in 375 ml. AcOH, left 15-16 hrs. at room temperature, evaporated, the residue poured into ice-H2O, and the solid extracted with Et2O gave 34.36 g. 2-amino-3,5-dibromopyrazine (II), m. 114°. II (7 g.) refluxed 9 hrs. in MeOH-NaOMe gave 5.4 g. 2-amino-3-methoxy-5-bromopyrazine (III), m. 138°. III (3 g.) hydrogenated in MeOH with H over Pd-C and KOH gave 1.5 g. 2-amino-3-methoxypyrazine (IIIa), m. 85°. p-Acetamidobenzenesulfonyl chloride (2.9 g.) added during 0.5 hr. to 2.5 g. III in 30 ml. anhydrous C5H6N, the mixture kept 20 hrs. at room temperature, heated 6 hrs. at 60°, and evaporated gave 3.7 g. 2-(p-acetamidobenzenesulfonamido)-3-methoxy-5-bromopyrazine (IV), m. 230-3°. IV (2.14 g.) and 10 ml. 10% NaOH refluxed 1 hr. gave 1.7 g. 2-sulfanilamido-3-methoxy-5-bromopyrazine, m. 212-13°. IIIa (1.5 g.) gave 2.21 g. 2-(p-acetamidobenzenesulfonamido)3-methoxypyrazine

(V), m. 224° 2-sulfanilamido-3-methoxypyrazine m. 175°. 2-Carboxyamino-3-hydroxypyrazine (20 g.) and 85 ml. POCl3 heated 2 hrs. at 100° gave 14 g. 2-cyano-3-chloropyrazine (VI), m. 48°. VI (19 g.) refluxed 2-3 hrs. with MeOH-NaOMe gave 16.5 g. 2-cyano-3-methoxypyrazine (VII), m. 56°. VII (10 g.) and 140 ml. 5% H2O2 made alkaline with 2N NaOH kept 4 hrs. at 50-5° gave 9 g. 2-carboxyamino-3-methoxypyrazine (VIII), m. 146°. VIII (5.4 g.) stirred 2 hrs. at 80° with NaOBr solution gave 3.13 g. IIIa. 2-Amino-3-chloropyrazine (70 mg.) refluxed 12 hrs. with NaOMe-MeOH gave the theoretical yield of IIIa. p-Nitrobenzenesulfonyl chloride (44.4 g.) added in 20-30 min. to 25 g. IIIa in 200 ml. anhydrous C6H5N, stirred 24 hrs. at room temperature, and warmed 8-10 hrs. at 60° gave 50 g. 2-(p-nitrobenzenesulfonamido)-3-methoxypyrazine (IX), m. 197°. IX (38 g.) kept 45-60 min. at 95° with 83 ml. C5H5N and 33.5 ml. Ac2O gave 40 g. 2-(N-acetyl-p-nitrobenzenesulfonamido)-3-methoxypyrazine (X), m. 187° (alc.-Me3CO). X (7 g.) in 120 ml. dioxane hydrogenated at room temperature and atmospheric pressure over 5 g. 10% Pd-C for 8-9 hrs. gave 3 g. 2-(N-acetylsulfanilamido)-3-methoxypyrazine, m. 190-5°. 2-[Bis(p-acetamidobenzenesulfonamido)]-3-chloropyrazine (Xa) (26 g.) and 10.4 g. NaOH in 70 ml. H2O heated 2 hrs. gave 75% 2-(p-aminobenzenesulfonamido)-3-chloropyrazine (XI), m. 156-8°. XI (6 g.) and 1.2 g. Na in 100 ml. MeOH heated 15 hrs. at 110° gave 86% 3-methoxysulfapyrazine (XII), m. 168-72°. Xa (26 g.) heated 15 hrs. at 120° with NaOMe-MeOH gave 82% XII. The pharmacol. data of some of the sulfapyrazines of this invention were given in 6 tables.

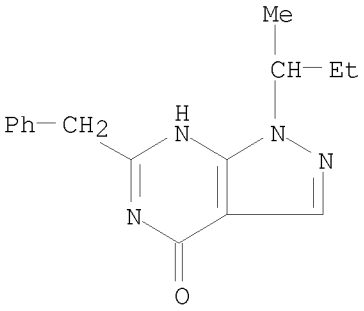
L4 ANSWER 42 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:469189 CAPLUS
DOCUMENT NUMBER: 59:69189
ORIGINAL REFERENCE NO.: 59:12820a-h,12821a
TITLE: Pyrazolo[3,4-d]pyrimidines
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1149013		19630522	DE	
PRIORITY APPLN. INFO.:			CH	19600511

IT 5494-84-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5494-84-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



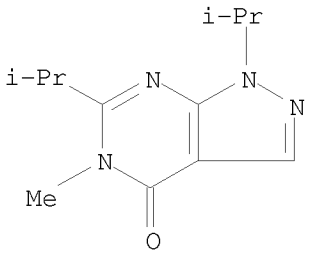
IT 93022-43-6P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Pyrazolo[3,4-d]pyrimidines)
RN 93022-43-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylpropyl)-6-(phenylmethyl)- (CA INDEX NAME)



IT 1143-77-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,

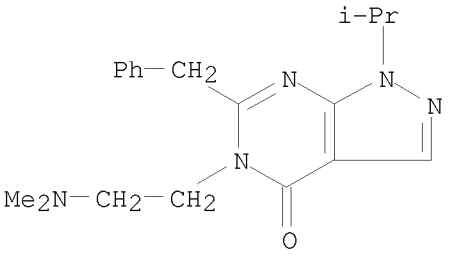
1,5-dihydro-1,6-diisopropyl-5-methyl- 1168-08-7P,
4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-isopropyl-
1168-43-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-
1168-44-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-, hydrochloride
1173-93-9P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[3-(diethylamino)propyl]-1,5-dihydro-1-isopropyl-
1173-94-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[3-(diethylamino)propyl]-1,5-dihydro-1-isopropyl-,
hydrochloride 1180-45-6P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-6-(diphenylmethyl)-1,5-dihydro-1-isopropyl-
1229-51-2P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-1,5-dihydro-1-isopropyl-5-methyl- 1237-01-0P,
4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1,6-diisopropyl- 1242-91-7P
, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-isopropyl-,
hydrochloride 1248-41-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-isopropyl-, hydrochloride
1254-49-5P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-
5494-82-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 1,6-diisopropyl-
91803-32-6P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-methyl-
93022-44-7P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-benzyl-1-isobutyl- 94331-62-1P,
1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-phenyl- 95225-07-3P
, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-isobutyl-
96001-11-5P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol,
6-(diphenylmethyl)-1-isopropyl- 100321-66-2P,
4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-isobutyl-, hydrochloride
101405-08-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-benzyl-5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-, hydrochloride
RL: PREP (Preparation)
(preparation of)

RN 1143-77-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-5-methyl-1,6-bis(1-methylethyl)- (CA INDEX NAME)

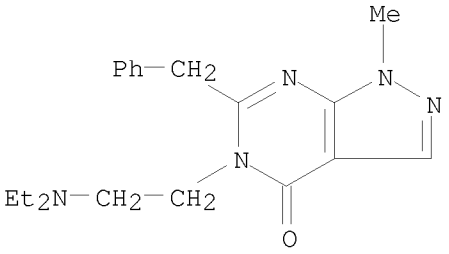


RN 1168-08-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-

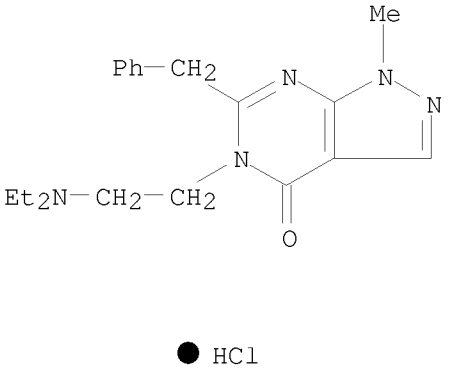
(CA INDEX NAME)



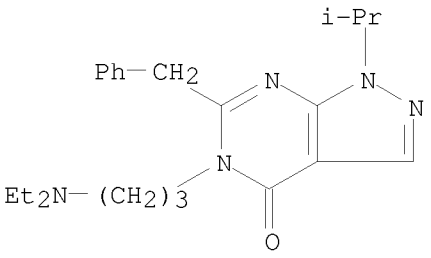
RN 1168-43-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-6-(phenylmethyl)- (CA
INDEX NAME)



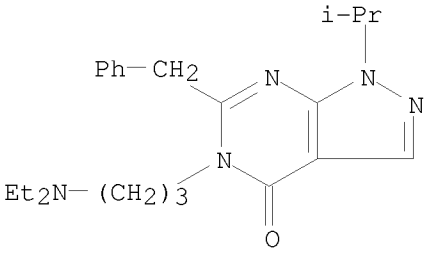
RN 1168-44-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-methyl-6-(phenylmethyl)-,
hydrochloride (1:1) (CA INDEX NAME)



RN 1173-93-9 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[3-(diethylamino)propyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-
(CA INDEX NAME)

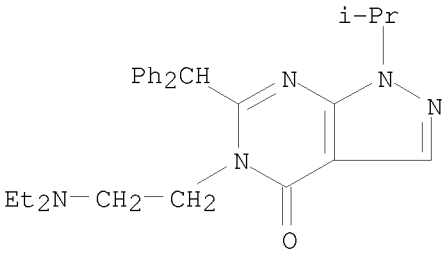


RN 1173-94-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[3-(diethylamino)propyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-
, hydrochloride (1:1) (CA INDEX NAME)

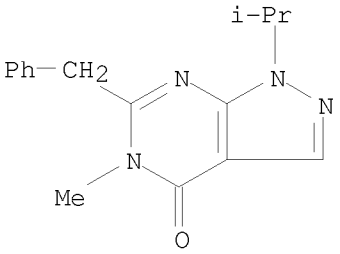


● HCl

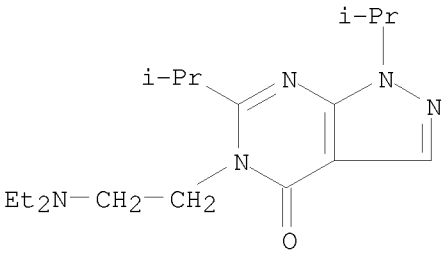
RN 1180-45-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-6-(diphenylmethyl)-1,5-dihydro-1-(1-methylethyl)-
(CA INDEX NAME)



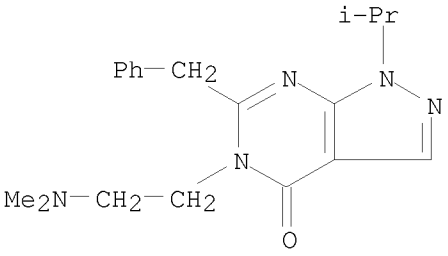
RN 1229-51-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-5-methyl-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



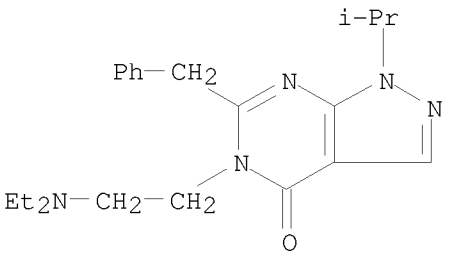
RN 1237-01-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1,6-bis(1-methylethyl)- (CA INDEX NAME)



RN 1242-91-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-, hydrochloride (1:1) (CA INDEX NAME)

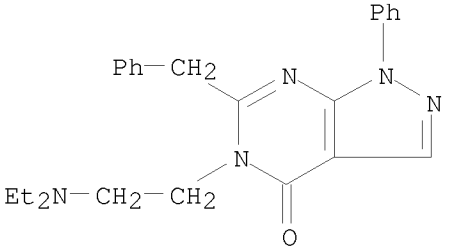


RN 1248-41-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)-, hydrochloride (1:1) (CA INDEX NAME)

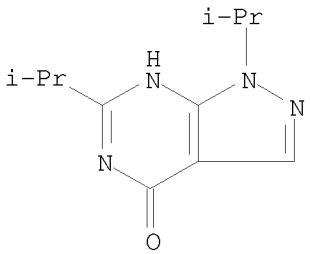


● HCl

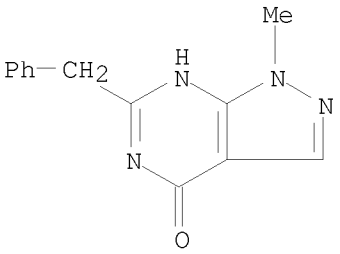
RN 1254-49-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



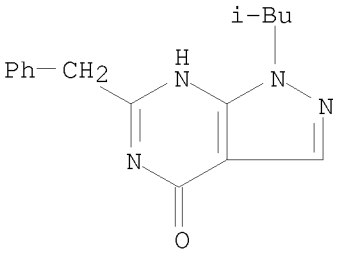
RN 5494-82-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1,6-bis(1-methylethyl)- (CA INDEX NAME)



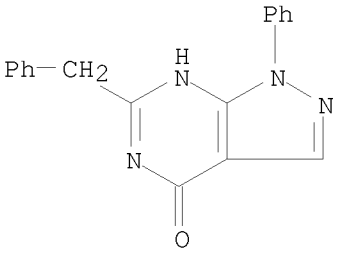
RN 91803-32-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(phenylmethyl)- (CA INDEX NAME)



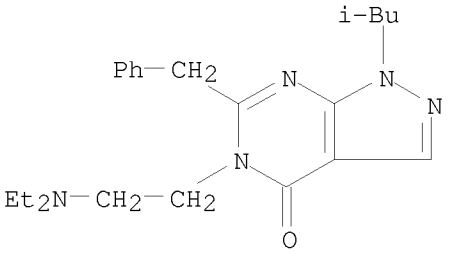
RN 93022-44-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)- (CA INDEX NAME)



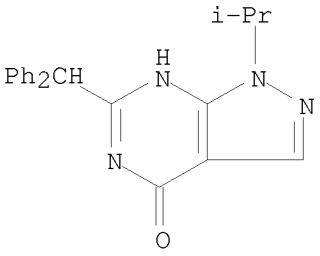
RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)-
(CA INDEX NAME)



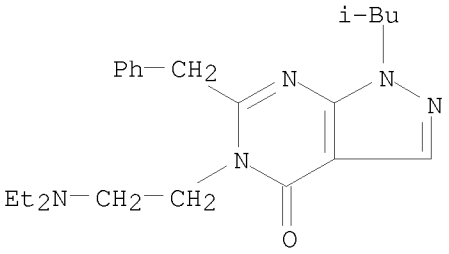
RN 95225-07-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)-
(CA INDEX NAME)



RN 96001-11-5 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-(diphenylmethyl)-1,5-dihydro-1-(1-methylethyl)- (CA INDEX NAME)

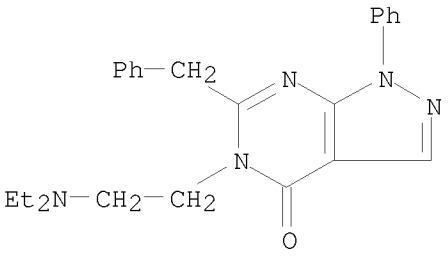


RN 100321-66-2 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)-
, hydrochloride (1:?) (CA INDEX NAME)



●x HCl

RN 101405-08-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
5-[2-(diethylamino)ethyl]-1,5-dihydro-1-phenyl-6-(phenylmethyl)-,
hydrochloride (1:?) (CA INDEX NAME)



●x HCl

GI For diagram(s), see printed CA Issue.

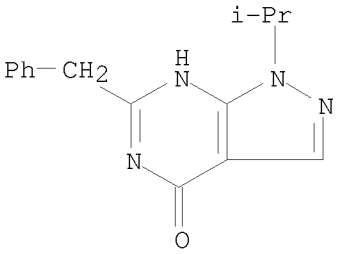
AB 4-Oxo-4,5-dihydropyrazolo[3,4-d]pyrimidines (I), possessing vasodilating ability, are described in which R1 = H, alkyl or phenyl group, R2 = H or lower alkyl group, R3 = HO, halogen, NR5R6 (R5 and R6 = H, alkyl groups or joined together through O, S, or N) (or the position may be unsubstituted), R4 = alkyl or aralkyl group. The most active compds., I (R1 = iso-Pr, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (II) and I (R1 = sec-Bu, R2 = H, R3 = Et2NCH2CH2, R4 = PhCH2) (III) at a concentration of 10 γ/ml. increase coronary blood flow 78-73% in the Langendorf isolated dog heart procedure. In the same test, 1-isopropyl-4-diethylaminopyrazolo-[3,4-d]pyrimidine (CA 55, 13457a) at the same concentration causes an increase of 60%. In the compds. described below R2 = H. Na (2.3 g.) is finely dispersed in 50 ml. PhCH2CN and 9.9 g. 2-isopropyl-3-amino-4-carbethoxypyrazole (IV) added. The mixture is heated to 110-20° with stirring for 4 hrs. and cooled, 100 ml. alc. is added, and the mixture evaporated to dryness in vacuo. The residue is taken into 150 ml. 2N NaOH, extracted with CHCl3 to remove undissolved material and adjusted to pH 5 to 6 with 6N HCl to yield 1-isopropyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (V), m. 165-6° (alc.). V in 30 ml. N NaOH treated with Me2SO4 gave I (R1 = iso-Pr, R3 = Me, R4 = PhCH2) (VI), m. 96-7°. The procedure similar to that used for the preparation of IV is used to prepare 1-sec-butyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (VII), m. 154-5°. A solution of 1.15 g. Na in 40 ml. absolute alc. is added to 14.4 g. VII in 60 ml. absolute alc. and refluxed 4 hrs. after the addition of 7.5 g. Et2NCH2CH2Cl to give after HCl treatment 15.4 g. III.HCl, m. 147-8°. Similarly, 13.4 g. V is allowed to react with 1.2 g. Na in 300 ml. absolute EtOH, then with 5.5 g. Me2NCH2CH2Cl to yield 10.2 g. I (R1 = iso-Pr, R3 = Me2NCH2CH2, R4 = PhCH2) (VIII), m. 115-17°; VIII.HCl m. 229-31°. V, as the Na salt, is allowed to react with Et2NCH2CH2Cl to yield I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = PhCH2).HCl, m. 202-3°. When V, as the Na salt, is allowed to react with Et2NCH2CH2CHCl, II.HCl, m. 173-5°, is isolated. 1-Methyl-4-hydroxy-6-benzylpyrazolo[3,4-d]pyrimidine (IX) is prepared from 2-methyl-3-amino-4-carbethoxypyrazole and PhCH2CN (X) by the procedure for the preparation of V. The reaction of 12 g. IX with 1.2 g. Na in 25 ml. absolute alc. followed by the addition of 6 g. Et2NCH2CH2Cl leads to the isolation of I (R1 = Me, R3 = Et2NCH2CH2, R4 = PhCH2) (XI), m. 83-5° XI.HCl m. 219°. Likewise, 2-phenyl-3-amino-4-carbethoxypyrazole and X yields

1-phenyl-6-benzyl-4-hydroxypyrazolo[3,4-d]pyrimidine, m. 264-5° which is allowed to react as the Na salt with Et2 NCH2CH2Cl to give I (R1 = Ph, R3 =Et2NCH2CH2,CH2, R4 = PhCH2) (XII), m. 103 5° XII.HCl m. 225°. To an ice-cooled solution of 9.9 g. IV in 50 ml. MeCN is added 2.3 g. Na and the temperature of reaction kept below 30°. After the addition, the mixture is heated to 90-95° for 4 hrs., cooled, and 100 ml. EtOH added. The mixture is evaporated to dryness and residue treated with 150 ml. 2N NaOH, extracted with CHCl3 and the aqueous layer adjusted to pH 3 to 4 with 5N HCl and the precipitate crystallized from alc. to give 1-isopropyl-4-hydroxy-6-methylpyrazolo[3,4-d]pyrimidine (XIII), m. 195-6°. The reaction of 9.1 g. XII with 1.2 g. Na in 150 ml. absolute alc., followed by the addition of 7 g. Et2NCH2CH2Cl, and 4 hrs. reflux yields 7 g. I (R1 = iso-Pr, R3 = Et2NCH2CH2, R4 = Me), m. 166-8°. 1,6-Diisopropyl-4-hydroxypyrazolo[3,4-d]pyrimidine (XIV), m. 175-7°, is prepared from iso-BuCN and IV in the presence of Na. A solution of 11 g. XIV in 75 ml. 2N NaOH solution is stirred at room temperature with 6.3 g. Me2SO4 and allowed to stand overnight to yield 9 g. I (R1 = R4 = iso-Pr, R3 = Me), m. 175-7°. XIV (10 g.) is added to a solution of 1.05 g. Na in 150 ml. absolute alc., stirred 1 hr. at room temperature and 6.5 g. Et2. NCH2CH2Cl is added. The mixture is refluxed 4 hrs., evaporated to dryness in vacuo and the residue dissolved in 100 ml. N HCl, adjusted to a pH with NaOH solution and the oil that results is extracted with Et2O. The residue, after removal of the Et2O, is distilled to yield 9 g. I (R1 = R4 = iso-Pr, R3 = Et2NCH2CH2), b0.05 138-40°. A mixture of 20 g. X and 19.7 g. IV is warmed to 70° and 2.3 g. of Na in small pieces added. The mixture is heated 4 hrs. at 110-20°, allowed to cool, and the excess Na destroyed by the addition of alc. The mixture is evaporated to dryness in vacuo, the residue treated with 300 ml. H2O and 2N HCl added to adjust the pH to 3. The precipitate is removed by filtration and crystallized from petr. ether to yield 1-isopropyl-4-hydroxy-6-diphenylmethylpyrazolo[3,4-d]pyrimidine (XV), m. 226 7°. XV(5.2 g.)is added to a solution of 0.35g. Na in 150 ml. EtOH, the mixture stirred at room temperature and 2.1 g. Et2NCH2CH2Cl is added. The mixture is refluxed 4 hrs. and evaporated to dryness in vacuo and the residue crystallized from petr. ether to yield 3.8 g. I (R1 = iso-Pr, R3;= Et2NCH2CH2, R4 = Ph2CH), m. 124-5°.

L4 ANSWER 43 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:469188 CAPLUS
DOCUMENT NUMBER: 59:69188
ORIGINAL REFERENCE NO.: 59:12819d-h,12820a
TITLE: 4H-Pyrido[1,2-a]pyrimidin-4-ones
INVENTOR(S): Allen, Robert E.
PATENT ASSIGNEE(S): Cutter Laboratories, Inc.
SOURCE: 27 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 621702		19621214	BE	
FR M2201			FR	
GB 970439			GB	
US 3149112		1964	US	
PRIORITY APPLN. INFO.:			US	19610906

OTHER SOURCE(S): MARPAT 59:69188
IT 5494-84-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5494-84-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



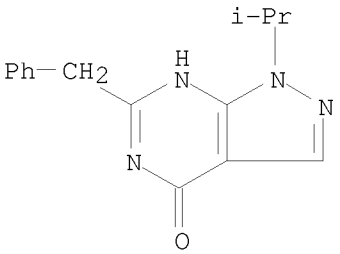
AB The title compds. (I) (A is an alkylene group, NR2 is dialkylamino, piperidino, morpholino, or pyrrolidino and R1 is alkyl, cycloalkyl, aryl, or arylalkyl) were made from II; a mixture of equimol. quantities of 2-aminopyridine and di-Et alkylmalonate was heated to >190° several hrs. The cooled, yellow reaction mixture was treated with Et2O. Thus were made the following II (R1 and m.p. given): Me, 305-10° (III); Et, 265-6°; Pr, 252-6°; iso-Bu, .apprx.235°; hexyl, 208-9°; octyl, 197-8°; decyl, 190-1°, cyclohexyl, 295° (decomposition); Ph, 308-10°; p-MeOC6H4, .apprx.320°; benzyl, 320° (decomposition); p-MeC6H4CH2, 320° (decomposition); p-ClC6H4CH2, .apprx.320°; p-MeOC6H4CH2, 300° (decomposition); p-EtOC6H4CH2, .apprx.288°; p-MeOC6H4(CH2)2, 257-8°; o-MeOC6H4CH2, 243°. Also prepared were 2-hydroxy-3,7-dimethyl-4H-pyrido[1,2-a]pyrimidin-4-one, m. 324-6°, and 2-hydroxy-3-(p-methoxybenzyl)-7-methyl-4H-pyrido[1,2-a]pyrimidin-4-one, m. 312° (decomposition). I was prepared from II as shown in this example: A solution of 24 g. Me2NCH2CH2Cl in 200 ml. toluene was added to a solution of 19 g. III and 5.9 g. MeONa in 150 ml. EtOH. The mixture was

refluxed, the alc. distilled, aqueous NaOH added, the organic layer dried, and the toluene distilled The oily amine, on treatment with EtOH saturated by HCl, gave I HCl salt [A = (CH2)2, R = R1 = Me], m. 215°. Similarly prepared were the following I HCl salts [A = (CH2)] (R, R1, and m.p. given): Et, H, 197-8° (decomposition); Et, Me, 207°; Et, Et, 160-1°; Me, Et, 176-9°; Me, Pr, 139-40°; Me, iso-Bu, 166°; Et, hexyl, 128°; Et, octyl, 90-120°; Me, decyl, 85-120°; Et, cyclohexyl, 188-9°; Et, Ph, 209-10°; Et, p-MeOC6H4, 217°; Et, benzyl, 167-73° (decomposition); Me, benzyl, 198-201°; Et, p-MeC6H4CH2, 206-8°; Et, p-ClC6H4CH2, 225° (decomposition); Et, p-MeOC6H4CH2, 196-7°; Me, p-MeOC6H4CH2, 172-3°; Et, p-EtOC6H4CH2, 222°; Et, p-MeOC6H4(CH2)2, 146-7°; Et, o-MeOC6H4CH2, 217°; iso-Pr, Me, 205-7°. Also prepared were these I HCl salts [A = (CH2)2] (NR2, R1, and m.p. given): piperidino, p-MeOC6H4CH2, 190-202°; morpholino, p-MeOC6H4CH2, 161-2°. Also made were these I HCl salts, with a Me group in position 7 (R, R1, and m.p. given): Me, p-MeOC6H4CH2, 207-8°; Me, p-MeOC6H4CH2, 161-5°; Et, Me, 214-15°. Also described was the HCl salt of 2-(2-dimethylaminopropoxy)-3-(p-methoxybenzyl)-4H-pyrido[1,2-a]pyrimidin-4-one, m. 182-5°. These I are stimulants of the central nervous system.

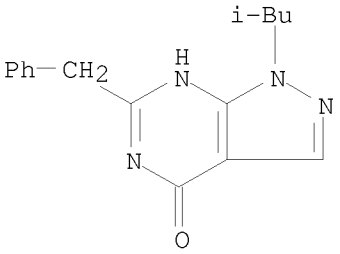
L4 ANSWER 44 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:462450 CAPLUS
DOCUMENT NUMBER: 59:62450
ORIGINAL REFERENCE NO.: 59:11529e-g
TITLE: 1 - Isopropyl- 4 - hydroxy - 6 - benzylpyrazolo [3,4 - d] pyrimidine
INVENTOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 5 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1147234		19630418	DE	
CH 390264			CH	
CH 398626			CH	
CH 403786			CH	
GB 937722			GB	
GB 937723			GB	
US 3165520		1965	US	
US 3169965		1965	US	
US 3211731		19651012	US 1961-107906	19610505
US 3211732		1965	US	
PRIORITY APPLN. INFO.:			CH	19600511

IT 5494-84-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5494-84-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



IT 93022-44-7P, 1H-Pyrazolo[3,4-d]pyrimidin-4-ol, 6-benzyl-1-isobutyl-
RL: PREP (Preparation)
(preparation of)
RN 93022-44-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(2-methylpropyl)-6-(phenylmethyl)- (CA INDEX NAME)



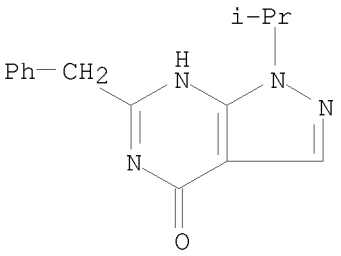
GI For diagram(s), see printed CA Issue.

AB The title compound (I), which exhibits coronary-dilating activity, was prepared by various methods. Thus, 2.3 g. Na was crushed in 50 cc. PhCH2CN (II), 9.9 g. 2-isopropyl-3-amino-4-carbethoxypyrazole added, the mixture heated to 110-20° for 4 hrs. by stirring, cooled, 100 cc. EtOH added, and evaporated in vacuo to dryness, the residue dissolved in 150 cc. 2N NaOH, extracted with CHCl3, the aqueous solution adjusted to pH 5-6 with 6N HCl, and the precipitate filtered off to give 6.2 g. I, m. 165-6° (EtOH). Similarly, I was prepared from 2-isopropyl-3-amino-4-carbamoylpyrazole (III) and II, from III and PhCH2CONH2, from 2-isopropyl-3-amino-4-carboxypyrazole via 2-isopropyl-3-(phenylacetamido)4-carboxypyrazole, m. 163-4°, and 1-isopropyl-4-oxo-6-benzylpyrazolo[3,4-d]oxazine, m. 100-1°, or from 2-isopropyl-3-amino-4-cyanopyrazole via 2-isopropyl-3-(phenylacetamido)-4-cyanopyrazole.

L4 ANSWER 45 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:462449 CAPLUS
DOCUMENT NUMBER: 59:62449
ORIGINAL REFERENCE NO.: 59:11529d-e
TITLE: Dipyridylium quaternary salts
INVENTOR(S): Jubb, Anthony H.
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

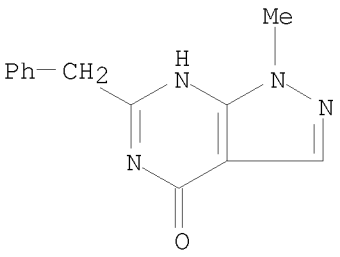
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 926326		19630515	GB 1959-28654	19590821
PRIORITY APPLN. INFO.:			GB	19590821

IT 5494-84-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5494-84-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)

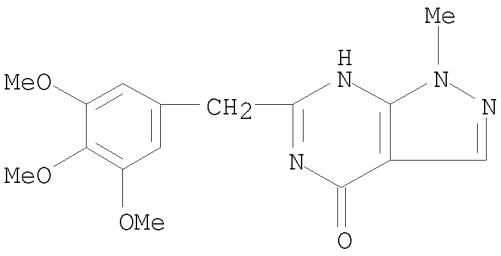


GI For diagram(s), see printed CA Issue.
AB The title compds. represented by I where X- = an anionic radical, were prepared by heating an excess of C2H4Br2 (II) with 2,2'-dipyridyl (III) at elevated pressures and at temps. above the b.p. of the diester. Thus, 3.98 g. III and 39.8 g. II was heated in a sealed tube for 7.5 hrs. at 170°. The formed 1,1'-ethylene-2,2'-dipyridylium dibromide, washed with Me2CO and dried at 100° weighed 8.65 g. (98%).

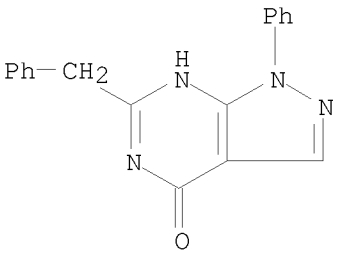
L4 ANSWER 46 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:408986 CAPLUS
DOCUMENT NUMBER: 59:8986
ORIGINAL REFERENCE NO.: 59:1635g-h
TITLE: New synthesis of pyrazolo[3,4-d]pyrimidines with dilatory effect on coronary vessels
AUTHOR(S): Schmidt, Paul; Eichenberger, Kurt; Wilhelm, Max; Burckhardt, Christoph A.
CORPORATE SOURCE: CIBA S. A., Basel, Switz.
SOURCE: Annali di Chimica (Rome, Italy) (1963), 53, 61-9
CODEN: ANCRAI; ISSN: 0003-4592
DOCUMENT TYPE: Journal
LANGUAGE: French
IT 91803-32-6P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-methyl- 93022-79-8P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(3,4,5-trimethoxybenzyl)- 94331-62-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 91803-32-6 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(phenylmethyl)- (CA INDEX NAME)



RN 93022-79-8 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-[(3,4,5-trimethoxyphenyl)methyl]- (CA INDEX NAME)

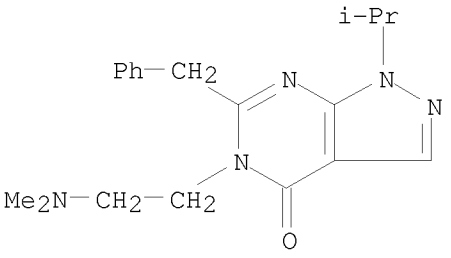


RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



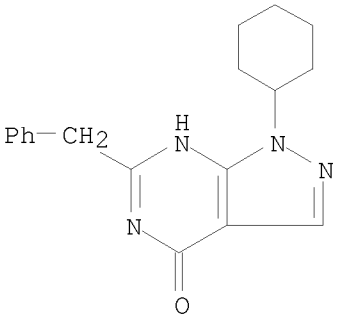
AB cf. Helv. Chim. Acta 45, 1620(1962). The position of the functional groups of 3-amino-4-carbethoxypyrazoles suggested the formation of bicyclic compds. by the action of appropriate reagents. Treatment with suitable nitriles led to a new synthesis of pyrazolo[3,4-d]pyrimidines substituted in the 6-positions, and to 6-aminopyrazolo[3,4-b]pyridines. The reaction was extended to numerous examples and the constitution of the products proved by independent syntheses (exptl. details, loc. cit.). Degradation in acid media converted the 6-substituted pyrazolopyrimidines to pyrazole derivs. Several of the compds. possessed a marked dilatory effect on the coronary vessels.

L4 ANSWER 47 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:483252 CAPLUS
DOCUMENT NUMBER: 57:83252
ORIGINAL REFERENCE NO.: 57:16612e-g
TITLE: Some bacterial pigments (phenazines)
AUTHOR(S): Holliman, F. G.
CORPORATE SOURCE: Univ. Cape Town, S. Afr.
SOURCE: South African Industrial Chemist (1961), 15(No. 12), 233-8
CODEN: SAICA8; ISSN: 0370-8225
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 1168-08-7
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 1168-08-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)

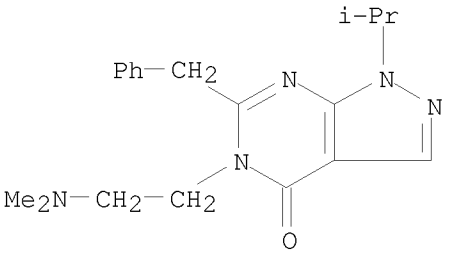


AB Two red pigments were obtained from Pseudomonas aeruginosa by elution from charcoal using a solution of pyridine in water. The bacteria were grown in mannitol and pigment production was very sensitive to O. The 2 pigments had empirical formulas of C15H15N3O4 (I) and C15H15N3O6S (II). The alkaline degradation product of I was shown to be 2-aminophenazine-6-carboxylic acid (III) by ultraviolet and infrared spectra and by subsequent synthesis of the material. Synthetic I was identical to the isolated pigment by paper chromatography, I.R., analysis, and x-ray diffraction. II had the same chromophore as I, but its identity was not established. The infrared spectrum and electrophoretic behavior of II suggested it to be a sulfonic acid.

L4 ANSWER 48 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:483251 CAPLUS
DOCUMENT NUMBER: 57:83251
ORIGINAL REFERENCE NO.: 57:16611d-i,16612a-e
TITLE: Chemotherapeutic studies in the heterocyclic series. XXXIV. Pyrazolopyrimidines. 5. A new synthesis of pyrazolo[3,4-d]pyrimidine with coronary dilating properties
AUTHOR(S): Schmidt, P.; Eichenberger, K.; Wilhelm, M.
CORPORATE SOURCE: Ciba, Basel, Switz.
SOURCE: Helvetica Chimica Acta (1962), 45, 1620-7
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 57:83251
IT 94068-86-7
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 94068-86-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclohexyl-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)



IT 1168-08-7P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-isopropyl- 5494-84-8P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-isopropyl- 91803-32-6P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-methyl- 92023-17-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(p-chlorobenzyl)-1,5-dihydro-1-methyl- 92193-40-3P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-(2-hydroxyethyl)- 93022-79-8P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-methyl-6-(3,4,5-trimethoxybenzyl)- 93726-25-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-(p-ethoxybenzyl)-1,5-dihydro-1-isopropyl- 94331-62-1P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1,5-dihydro-1-phenyl- 97433-46-0P, 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-benzyl-1-cyclopentyl-1,5-dihydro-
RL: PREP (Preparation)
(preparation of)
RN 1168-08-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-[2-(dimethylamino)ethyl]-1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



RN 5494-84-8 CAPLUS
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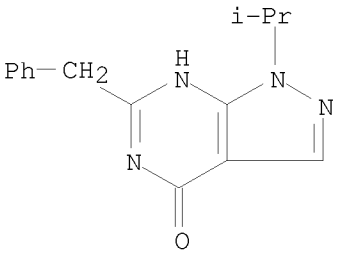
1,5-dihydro-1-(1-methylethyl)-6-(phenylmethyl)- (CA INDEX NAME)



RN 91803-32-6 CAPLUS
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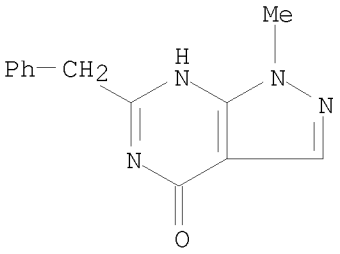
(CA INDEX NAME)



RN 92023-17-1 CAPLUS
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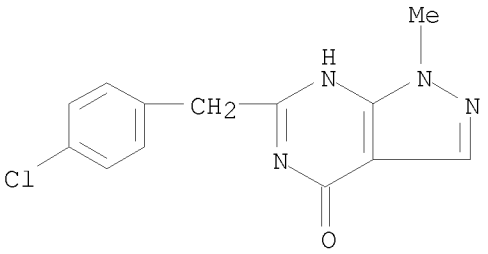
6-[(4-chlorophenyl)methyl]-1,5-dihydro-1-methyl- (CA INDEX NAME)



RN 92193-40-3 CAPLUS
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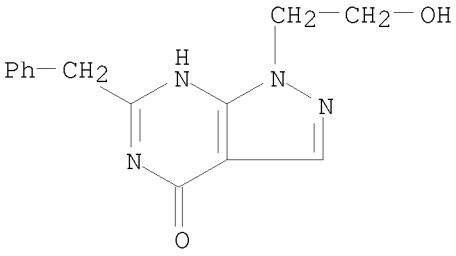
1,5-dihydro-1-(2-hydroxyethyl)-6-(phenylmethyl)- (CA INDEX NAME)



RN 93022-79-8 CAPLUS
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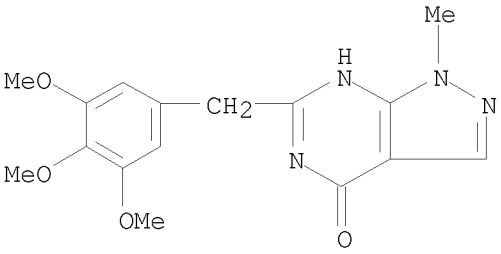
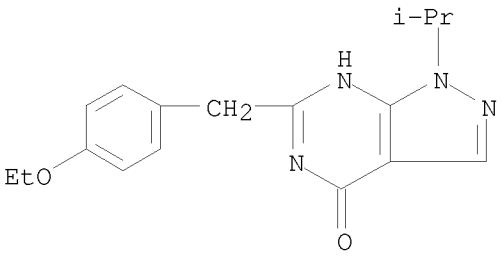
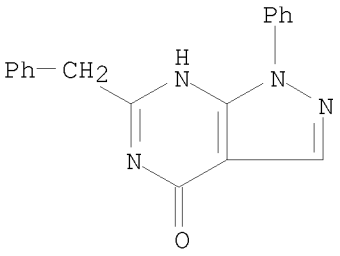
1,5-dihydro-1-methyl-6-[(3,4,5-trimethoxyphenyl)methyl]- (CA INDEX NAME)



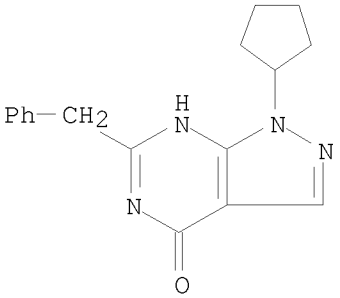
RN 93726-25-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one,
6-[(4-ethoxyphenyl)methyl]-1,5-dihydro-1-(1-methylethyl)- (CA INDEX NAME)



RN 94331-62-1 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-phenyl-6-(phenylmethyl)- (CA INDEX NAME)



RN 97433-46-0 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclopentyl-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)

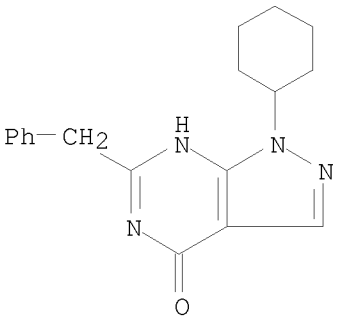


AB cf. CA 53, 20070d. The condensation of 3-amino-4-carbethoxypyrazoles with nitriles led to a new synthesis of 6-(C-substituted) pyrazolo[3,4-d]pyrimidines (I) and 6-aminopyrazolo[3,4-b]pyridines. The I could be cleaved with H3PO4 to 3-aminopyrazole-4-carboxamide derivs. Many of the new I caused an increase of coronary flow. 2-Isopropyl-3-amino-4-carbethoxypyrazole (II) (19.7 g.) in 250 cc. 2N NaOH refluxed 2 hrs., cooled, treated with C, and acidified with concentrated HCl to pH 3-4 gave 14.5 g. 4-CO2H analog (III) of II, m. 151-2° (decomposition). III (84.5 g.) in 375 cc. dioxane and 40 cc. C5H5N treated dropwise with stirring at 10-15° with 77.3 g. PhCH2COCl in 125 cc. dry dioxane, stirred 1 hr. at 10° and 2 hrs. at room temperature, diluted

with H2O and aqueous HCl, and extracted with Et2O gave 53 g. 2-isopropyl-3-phenylacetylamino-4-carboxypyrazole (IV), m. 162-3°. IV (8.61 g.) and 30 cc. Ac2O stirred 3 hrs. at 100-10° and evaporated yielded 3.1 g. 1-isopropyl-4-oxo-6-benzylpyrazolo[3,4-d]oxazine (V), m. 162-3° (Me2CO-petr. ether). III (30 g.) in 180 cc. dry dioxane and 16 cc. C5H5N treated dropwise with stirring at 10-15° with 31 g. PhCH2COCl in 50 cc. dioxane and processed in the usual manner gave 21 g. 4-CN analog (VI) of IV, m. 140-2° (EtOH). PhCH2CN (26.3 g.) in 250 cc. CHCl3 and 13 cc. absolute EtOH saturated with dry HCl, kept overnight, evaporated below 30°, the residue dissolved in 200 cc. CHCl3, treated with 16.9 g. 2-isopropyl-3-amino-4-carbamoylpyrazole (VII) in 1800 cc. CHCl3, refluxed 10 hrs. with stirring, filtered, and evaporated yielded 2-isopropyl-3-(1-ethoxy-2-phenylethylidenimino)-pyrazole-4-carboxamide (VIII), m. 111-14° (Et2O). II (70 g.) and 140 g. PhCH2CN added during 1 hr. with stirring at 90-5° to 16.5 g. powdered Na in 300 cc. dry MePh, refluxed 7 hrs. with stirring, diluted with 240 cc. absolute EtOH, evaporated, the residue dissolved in 1.2 1. N NaOH, washed with MePh, and acidified with 5N HCl to pH 5-6 gave 62.4 g. 1-isopropyl-4-oxo-6-benzyl-4,5 -dihydropyrazolo [3,4 - d]pyrimidine (IX), m. 164-6° (absolute EtOH); the alc. mother liquor concentrated, filtered, the residue (8.1 g.) shaken 0.5 hr. with 81 cc. CH2Cl2, and filtered left 4.77 g. 2-isopropyl-4-hydroxy-5-phenyl-6-aminopyrazolo[3,4-b]pyridine (X), m. 256-7° (EtOH); the CH2Cl2 filtrate evaporated gave 1.9 g. IX. Similarly were prepared the following 1,6-disubstituted-4-oxo-4,5-dihydropyrazolo[3,4-d]pyrimidines (1- and 6-substituent and m.p. given): Me, PhCH2, 233-7°; Me, p-ClC6H4CH2, 268-70°; Me, 3,4,5-(MeO)3C6H2CH2, 245-6°; HOCH2CH2, PhCH2, 194-5°; iso-Pr, Me, 180-2°; iso-Pr, Ph, 256-8°; iso-Pr, PhCH2, 165-6°; iso-Pr, p-EtOC6H4CH2, 175-6°; cyclopentyl, PhCH2, 189-90°; cyclohexyl, PhCH2, 207-8°; Ph, PhCH2 (XIII), 263-5°. V (5.4 g.), 50 cc. C6H6, and 15 cc. liquid NH3 in a sealed tube heated 8 hrs. at 100-10°, treated with 2N NaOH, and the aqueous phase acidified with 6N HCl to pH 6 gave 0.7 g. IX. VI(6.7g.) and 27.2 cc. 10% aqueous KOH in 102 cc. 3% H2O2 heated 10 hrs. at 70°, filtered, and acidified with 2N HCl to pH 5 yielded 6.12 g. IX, m. 163-5°. Crude VIII from 26.3 g. PhCH2CN and 16.9 g. VII added to 18 g. Na in 315 cc. MeOH, kept overnight, refluxed 0.5 hr., filtered, evaporated, the residue shaken with 200 cc. H2O and 200 cc. CHCl3, and the aqueous phase acidified with 5N HCl gave 16.6 g. IX. VII (8.4 g.) and 27 g. PhCH2CONH2 heated 4 hrs. at 200-10°, cooled, powdered, extracted with 2N NaOH, and the alkaline extract acidified with 2N HCl to pH 3 yielded 3.2 g. IX, m. 165-6° (EtOH). II (39.4 g.) in 150 cc. dry dioxane and 16 cc. C5H5N treated with stirring at 10-15° during 15 min. with 31 g. PhCH2COCl in 50 cc. dioxane, stirred 1 hr. at 10° and 2 hrs. at room temperature, treated with 130 cc. 2N HCl and 380 cc. H2O, and extracted with about 1000 cc. Et2O yielded 33 g. 2-isopropyl-3-phenylacetylamino-4-carbethoxypyrazole (XIV), b0.08 170-5°. NaNO2 (7 g.) and 26.8 g. X added successively with stirring at 0-5° to 268 cc. concentrated H2SO4, stirred 3 hrs. at 0-5°, cooled, poured onto ice, heated with stirring to 80°, cooled, filtered, the residue (about 20 g.) treated with 400 cc. saturated aqueous NaHCO3 and 400 cc. H2O, filtered, and the filtrate acidified with 2N HCl to pH 3-4 yielded 16.8 g. 1-isopropyl-4-hydroxy-5-phenyl- 6-oxo-4,5-dihydropyrazolo[3,4-b]pyridine

(XV), m. 322-4° (EtOH). XIV (10 g.) and 2 g. Na in 150 cc. MePh refluxed 5 hrs. with stirring, cooled to room temperature, treated with EtOH, evaporated, the residue dissolved in H2O, washed with Et2O, and acidified with 2N HCl gave 2.3 g. XV, m. 322-4° (aqueous EtOH). XIII (15 g.) and 100 cc. POCl3 refluxed 6 hrs., evaporated, the residue dissolved in CHCl3, and worked up gave 7.2 g. 1-phenyl-4-chloro-6-benzylpyrazolo[3,4-d]pyrimidine (XVI), m. 90-1° (CHCl3-petr. ether). XVI (7 g.) and 25 g. Me2NH in 50 cc. EtOH heated 7 hrs. at 100° in an autoclave gave 4.3 g. 4-Me2N analog of XVI, m. 121-2° (EtOH). IX (13.4 g.) and 1.15 g. Na in 300 cc. EtOH stirred 1 hr. at room temperature, treated with 5.5 g. Me2NCH2CH2Cl, refluxed 4 hrs., evaporated, the residue dissolved in 100 cc. N HCl, washed with Et2O, basified to pH 10 with aqueous NaOH, and extracted with Et2O yielded 13 g. 5-Me2NCH2CH2 derivative (XVII) of IX, m. 115-17° (petr. ether). XVII (10 g.) and 35 cc. 85% H3PO4 stirred 6 hrs. at 100°, poured onto 300 g. ice, adjusted with aqueous NaOH to pH 10, filtered, and extracted with CHCl3 gave 6 g. 2-isopropyl-3-aminopyrazole-4-carboxylic acid 2-dimethylaminoethylamide, m. 131-2° (iso-Pr2O).

L4 ANSWER 49 OF 50 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:483250 CAPLUS
DOCUMENT NUMBER: 57:83250
ORIGINAL REFERENCE NO.: 57:16609h-i,16610a-i,16611a-d
TITLE: Chemotherapeutic studies in the heterocyclic series. XXXIII. 1-Aryl-2-alkyl-3,6-dioxo-1,2,3,6-tetrahydropyridazines
AUTHOR(S): Druey, J.; Meier, Kd.; Staehelin, A.
CORPORATE SOURCE: Ciba, Basel, Switz.
SOURCE: Helvetica Chimica Acta (1962), 45, 1485-98
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 57:83250
IT 94068-86-7
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 94068-86-7 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-cyclohexyl-1,5-dihydro-6-(phenylmethyl)- (CA INDEX NAME)



AB cf. CA 57, 11157a. Several 1,2-disubstituted 3,6-dioxo-1,2,3,6-tetrahydropyridazines (I) were prepared Direct alkylation of 1-aryl-3-hydroxy-6-oxo-1,6-dihydropyridazines (II) with dialkyl sulfates gave either 1-aryl-2-alkyl-3,6-dioxo-1,2,3,6-tetrahydropyridazines (III) or a mixture of the III with the 3-alkyl ethers (IV) of II. Ph-NHNH2 (162 g.), 2.5 l. H2O, 365 g. 30% HCl, and 147 g. maleic anhydride (V) refluxed 4 h. with stirring, cooled to room temperature, and filtered yielded 225 g. yellowish crystalline 1-phenyl-3-hydroxy-6-oxo-1,6-dihydropyridazine, m. 262-3°. Similarly were prepared the following II (aryl group and m.p. given): p-MeC6H4 (VI) 242-4°, p-MeOC6H4 - (used crude), o-ClC6H4 (VII) 269-70°, m-ClC6H4 249-51°, p-ClC6H4 (VIII) 280-2°. II (100 g.) and 80 cc. Me2SO4 stirred 2.5 h. at 150°, stirred into 67.5 g. Na2CO3 in 1200 cc. H2O, stirred several hrs., and extracted with CHCl3 gave 96.1 g. 1-phenyl-2-methyl-3,6-dioxo-1,2,3,6 -tetrahydropyridazine (VIIIa), m. 173-5° (EtOAc-MeOH). Similarly were prepared the following I (2-substituent = Me) (1-substituent reaction time, reaction temperature and, m.p. given): p-MeC6H4, 132-4°, 5 h., 145-50°; p-MeOC6H4, 138.5-40°, 5-10 min., 190-200°; o-ClC6H4, 107-8°, 10 min., 190-200°; m-ClC6H4, 139-41°, 4 h., 150-5°; p-ClC6H4, 145-6°, 35 min., 150-200°. In the same manner were obtained the following 4(or 5)-substituted III (aryl = Ph, alkyl = Me) (substituent, m.p., reaction time, and reaction temperature

given): 4-MeO, 118.5-19.5°, 0.5 h., 140-50° [and the 3-Me ether of the 4-MeO derivative of II (aryl = Ph), m. 157-8°], 4-Me, 111-13°, 1.5 h., 140-50° [and the 3-Me ether of the 4-Me derivative of II (aryl = Ph), m. 117-18°]; 4-Cl, 150-2°, 3.5 h., 140-50°; 5-MeO, 156.5-7.5°, 4 h., 140-5°; 5-Me, 129-31°, 10 min., 190-200°; 5-Cl, 156-7.5°, 3.5 h., 140-50°. 1-Phenyl-3-hydroxy-4-chloro-6-oxo-1,6-dihydropyridazine (IX) (23 g.) in 300 cc. boiling MeOH treated dropwise during 45 min. with 9.2 g. Na in 200 cc. MeOH, refluxed 8 h., diluted with H2O, concentrated, filtered through C, acidified with AcOH, and cooled gave 18.4 g. 4-Me ether of IX, m. 260-2° (decomposition) (EtOH). 1-Phenyl-3-hydroxy-5-chloro-6-oxo-1,6-dihydropyridazine (X) (3.5 g.), 1 g. Na, and 100 cc. absolute MeOH heated 12 h. at 120-30° in a sealed tube, evaporated, the residue treated with 2N HCl, and filtered gave 2.2 g. 5-Me ether of X, m. 244-7° (MeOH). II (300 g.) and 300 cc. Et2SO4 heated 15 min. at 190-200°, cooled, stirred into 2 l. saturated aqueous Na2CO3, diluted with 2 l. H2O, stirred 4 h., and extracted with Et2O gave 120 g. (crude) 3-Et ether (XI) of II, m. 86-7° (EtOH); the aqueous phase extracted with CHCl3 gave 126 g. 1-phenyl-2-ethyl-3,6-dioxo-1,2,3,6-tetrahydropyridazine (XII), m. 121-3° (cyclohexane); the alkaline aqueous mother liquor acidified gave 50 g. unchanged II. Similarly were prepared the following IV and III (R = Et) (aryl group and m.p. of IV and III given): o-ClC6H4, 114-16°, 100-2°; p-ClC6H4, 141-2°, 142.5-43°; p-MeC6H4, 108-10°, 119-21°. MeNHNHPh.HCl (XIII.HCl) (9 g.) and 5.6 g. V in 60 cc. H2O heated with stirring on the water bath to solution, kept 3 days at room temperature, and extracted with CHCl3 yielded 1.7 g. VIIIa; the aqueous phase basified and extracted with Et2O yielded 4.6 g. unreacted XIII. Maleic acid mono-N-methyl-N'-phenylhydrazide (XIV) (10 g.) in 80 cc. Ac2O refluxed 0.5 h. gave 7.3 g. pale yellow crystalline II, m. 178-9.5° (MeOH). XIV (10 g.) in 100 cc. 33% HCl-MeOH kept 5 days at room temperature, evaporated, the residue treated with H2O, and extracted with CHCl3 gave 8.6 g. II, m. 173-6°. VIIIa (100 g.) in 1.4 l. absolute EtOH hydrogenated 20 min. at 40° over 10 g. Raney Ni gave 96.2 g. 1-phenyl-2-methyl-3,6-dioxohexahydropyridazine (XV), m. 143-5° (4:1 MeOH-H2O). HO2CCH2CH2CONMeNHPh (5 g.) in 10 cc. Ac2O refluxed 2 h., cooled, poured into H2O, kept 4 h., and filtered yielded 2.7 g. XV, m. 144-7.5°; 2.0 g. 2nd crop. VIIIa (2050 g.) in 3000 cc. AcOH treated during 1 h. at 80-5° with stirring with 1620 g. Br in 100 cc. AcOH, kept several hrs. at 5°, and filtered yielded 3176 g. 1-phenyl-2-methyl-3,6-dioxo-4,5-dibromohexahydropyridazine (XVI), m. 177-8.5° (decomposition) (MeOH). XVI (108 g.) and 35.5 g. C5H5N in 370 cc. CHCl3 refluxed 6 h. gave 81 g. (crude) 1-phenyl-2-methyl-5-bromo-3,6-dioxo-1,2,3,6 -tetrahydropyridazine (XVII), m. 159-61° (MeOH). VIIIa (15 g.) in 200 cc. AcOH stirred 2.5 h. on the water bath while being treated with Cl, the mixture evaporated, the residue diluted with H2O, and extracted with CHCl3 yielded 4.1 g. 4,5-di-Cl analog (XVIII) of XVI, m. 134-6° (MeOH). XVIII (0.9 g.) and 0.5 g. C5H5N in 15 cc. CHCl3 refluxed 6 h. yielded 0.75 g. 5-Cl analog (XIX) of XVII, m. 154-6° (MeOH). VIIIa (10.1 g.) in 250 cc. dry dioxane and 100 cc. MePh kept 4 wk at room temperature with 13 g. cyclopentadiene and a trace methylene blue, evaporated, and the residue (14.8 g.) recrystd. from MeOH gave 5.9 g. 2-phenyl-3-methyl-5,8-endomethylene-1,4-dioxo-1,2,3,4,4a,5,8,8a-

octahydrophthalazine, m. 127-7.5°. VIIIa (202 g.) in 1 l. 2N HCl refluxed 12 h., cooled, filtered from 60.3 g. fumaric acid, m. 285-7°, and extracted with $CHCl_3$ gave 27.2 g. unreacted VIIIa; the aqueous phase basified with cooling with 10N NaOH and extracted with Et_2O yielded 86.5 g. (crude) XIII, leaflets, m. 164-7° (absolute EtOH-Et_2O). VIIIa (101 g.) added with stirring at 30-5° to 20 g. NaOH in 500 cc. H_2O, stirred 4 h., filtered, the filtrate extracted with $CHCl_3$, and the extract evaporated gave 3.3 g. unreacted VIIIa; the filter residue dissolved at 30-40° with stirring in the $CHCl_3$-extracted filtrate and acidified with 6N HCl gave 84.6 g. XIV, m. 105-7° (EtOAc-petr. ether). XIII (6.1 g.) and 4.9 g. V in 50 cc. $CHCl_3$ kept several hrs. at room temperature, extracted with 2N aqueous Na_2CO_3, the extract acidified with 6N HCl, and extracted with $CHCl_3$ gave 7.0 g. VIIIa, m. 106-9°. XV (10.2 g.), 2.0 g. NaOH, and 150 cc. H_2O stirred 4 h. at room temperature and extracted with Et_2O gave 0.2 g. unchanged XV; the aqueous phase acidified and extracted with $CHCl_3$ yielded 10.5 g. (crude) XIV, m. 126-8°. XIV (44 g.) in 1 l. absolute EtOH hydrogenated under ambient conditions over 5 g. Raney Ni gave 40.5 g. XV, m. 124-6°. XV (10 g.) in 80 cc. morpholine refluxed 6 h. gave 15.5 g. morpholide of XV, m. 99-101° (Me_2CO-petr. ether). XV (20 g.) and 150 cc. liquid Me_2NH heated 6 h. in a sealed tube at 100-10° gave 25.3 g. (crude) dimethylamide of XV, m. 98-100° (Me_2CO-petr. ether). XV (5 g.) and 20 cc. $N_2H_4.HCO$ refluxed 6 h., evaporated, the residue diluted with H_2O, and extracted with $CHCl_3$ gave 1.5 g. XIII, m. 160-2°; the aqueous phase evaporated gave 2.2 g. $(CH_2CONHNH_2)_2$, m. 164-6° (aqueous EtOH). XVII (562 g.) and 84 g. NaOH in 4 l. H_2O stirred 4 h. at room temperature, filtered, and extracted with $CHCl_3$ gave 64 g. unreacted XVII, m. 224-6° (decomposition); the filtrate concentrated gave 515 g. Na salt (XX) of β-bromomaleic acid mono-N-methyl-N'-phenylhydrazide (XXI); the aqueous mother liquor acidified with HCl gave 26 g. 1-phenyl-2-methyl-3-pyrazolone-5-carboxylic acid (XXII), m. 198-200° (absolute EtOH). XX in H_2O acidified with HCl gave XXI, m. 135-7° (decomposition) (EtOAc). XX (215 g.) and 120 g. morpholine in 860 cc. H_2O refluxed 1.5 h., filtered hot, and acidified with HCl gave 131 g. XXII, m. 200.5-2.5° (decomposition) (absolute EtOH).

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ACCESSION NUMBER: 1958:88115 CAPLUS
DOCUMENT NUMBER: 52:88115
ORIGINAL REFERENCE NO.: 52:15540i,15541a-i,15542a-i,15543a-i
TITLE: Potential purine antagonists. VII. Synthesis of 6-alkylpyrazolo[3,4-d]pyrimidines
AUTHOR(S): Cheng, C. C.; Robins, Roland K.
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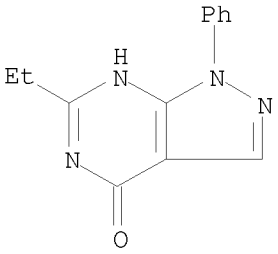
RL: PREP (Preparation)
(preparation of)
RN 5394-42-3 CAPLUS
CN 4H-Pyrazolo[3,4-d]pyrimidin-4-one, 6-ethyl-1,5-dihydro-1-phenyl- (CA INDEX NAME)



RN 100396-57-4 CAPLUS
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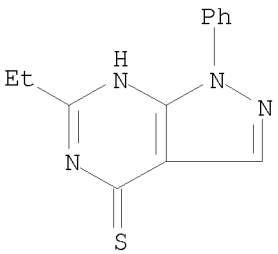

GI For diagram(s), see printed CA Issue.
AB cf. C.A. 52, 13741h. A synthesis of 6-alkyl-4-hydroxypyrazolo[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:COH (I) was devised from the corresponding 5-acylamino-4-cyanopyrazoles, R3CONHC:C(CN).CR2:N.NR1 (II) which were in turn prepared from 5-amino-4-cyanopyrazoles, R1N.N:CH.C(CN):CNH2 (III). Evidence was presented to show that the 5-acylaminopyrazole-4-carboxamide is an intermediate in this cyclization. Chlorination of I yielded the corresponding 6-alkyl-4-chloropyrazolo

[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CCl (IV). Nucleophilic displacement of the Cl in IV resulted in the preparation of a large number of 6-alkylpyrazolo[3,4-d]pyrimidines, R1N.N:CH.C:C.N:CR2.N:CNR4R5 (V). III (R1 = 3-Me) (80 g.) and 250 ml. Ac2O refluxed 10 hrs., excess Ac2O distilled in vacuo, the sirupy substance poured into 30 ml. C6H6, stirred several min., and crystallized gave 89 g. II (R1 = R2 = H, R3 = Me), crystals from H2O. Similarly II (R1 = R3 = Me, R2 = H) was prepared and the product recrystd. from H2O to a white powder. III (R1 = Ph) (150 g.) treated 19 hrs. under reflux with 200 ml. Ac2O, excess solvent removed, the residue treated with a small amount of C6H6, and Skellysolve (b. 60°), and the product isolated gave 171 g. II (R1 = Ph, R2 = H, R3 = Me) crystallized from H2O. The following II were thus prepared (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, H, Me, 221-2°, 76, H2O; Me, H, Me, 210-11°, 72, H2O; Ph, H, Me, 155-6°, 92, H2O; o-ClC6H4, H, Me, 175-5.5°, 82, alc., H2O; p-ClC6H4, H, Me, 173-5°, 96, alc, H2O; p-BrC6H4, H, Me, 175-5° (sic), 98, alc., H2O; p-O2NC6H4, H, Me, 198-200°, 95, alc., H2O; p-MeC6H4, H, Me, 128°, 96, alc., H2O; AcOCH2CH2, H, Me, 155-7°, 81, alc. II (R1 = Ph, R2 = H, R3 = Me) (30 g.) added at 15-20° to 120 ml. concentrated H2SO4, the clear solution stirred 0.5 hr., then poured onto 1 kg. ice, neutralized with concentrated NH4OH, the solid collected, washed, dried, and recrystd. from C6H6 and MeOH gave 20 g. 5-amino-1-phenylpyrazole-4-carboxamide (VI), m. 172-5°, identical with the product obtained from the hydrolysis of 5-amino-4-cyano-1-phenylpyrazole. VI (20 g.) and 200 ml. Ac2O refluxed 15 hrs., and purification gave 15 g. 6-methyl-4-oxo-1-phenylpyrazolo [3,4-d]-5,7-oxazine (VII), m. 184.5-5.5° (sublimed at 145°) (C6H6-C7H16). VII (2.5 g.) kept 2 hrs. at room temperature with 200 ml. H2O and 2 g. KOH, heated 10 hrs., acidified, and the precipitate collected gave 2 g. 5-acetamido-1-phenylpyrazole-4-carboxylic acid (VIII), m. 201-2° (AcOH), readily lost CO2 on heating. The 5-acetylamido group was retained in warm alkaline solution but hydrolyzed readily in cold acidic medium. VII (2 g.) left 0.5 hr. at room temperature with 100 ml. alc. NH3, heated briefly until a solid product precipitated, and the product collected gave 5-acetamido-1-phenylpyrazole-4-carboxamide (IX), m. 301-2°, relatively unstable. The m.p. of IX was the same as that for I (R1 = Ph, R2 = Me) and was undepressed in mixed m.p. The ultraviolet absorptions for IX at 230 mμ and for I at 233 and 269 mμ, were different. Thus IX cyclized at elevated temps. during the m.p. determination I were prepared by the following method. II (R1 = R2 = H, R3 = Me) (1.5 g.); 7 ml. 10% KOH, and 15 ml. 3% H2O2 warmed 0.5 hr. at 70-5°, the mixture acidified, the solid collected, and repptd. with dilute KOH and AcOH gave 1.1 g. I (R1 = H, R2 = Me). II (R1 = R3 = Me, R2 = H) (121 g.) warmed 10 hrs. at 70° with 1500 ml. 3% H2O2 and 400 ml. 10% KOH gave 103 g. I (R1 = R2 = Me), needles, sublimed at 180°. II (R1 = Ph, R2 = H, R3 = Me) (14.5 g.) in 5 g. KOH and 200 ml. 3% H2O2 warmed 5 hrs. at 70-5° and acidified gave 14 g. crude I (R1 = Ph, R2 = Me), m. 298-300°. IX(1 g.) heated 20 min. at 70° with 100 ml. 10% KOH, then acidified, the solid collected and recrystd. gave 0.8 g. product identical with that from the preceding experiment I (R1 = R2 = Me) (25 g.) and 400 ml. POCl3 refluxed 2 hrs., excess solvent removed, the sirup poured onto 1 kg. ice, the suspension left 15 min., extracted with CHCl3, dried, solvent removed at room temperature, and the solid isolated gave 24 g. IV (R1 = R2 = Me) as needles. I

(R1 = H, R2 = Me)(50 g.) refluxed 2 hrs. with 140 ml. PhNMe2 and 1 l. POCl3, excess POCl3 removed, the residue poured on ice, and extracted with Et2O gave 35 g. IV (R1 = H, R2 = Me), unstable. I (R1 = p-O2NC6H4, R2 = Me) (20 g.) refluxed 3 hrs. with 250 ml. POCl3 gave 17.5 g. IV (R1 = p-O2NC6H4, R2 = Me) as a yellow powder. Preparation of 1-alkyl(aryl)-6-alkyl-4-mercaptopyrazolo[3,4-d]pyrimidines X) (R1 = 1-substituent, R2 = 6-substituent) was achieved by the following two methods: (method 1) I (R1 = Ph, R2 = Me) (11 g.) and 50 g. P2S6 added portionwise during 45 min. to 400 ml. Tetralin (preheated to 165°), the temperature allowed to rise to 185°, then heated 6 hrs. to 190-5°, the solution cooled overnight, filtered, the product dissolved in dilute KOH and precipitated with AcOH gave 5.5 g. X (R1 = Ph, R2 = Me); method 2) IV (R1 = Ph, R2 = Me) (14 g.) and 14 g. CS(CH2)2 in 120 ml. alc. refluxed 4 hrs., the product collected and washed well with alc. and H2O, and the product purified by precipitation from a hot basic solution with AcOH gave 11.5 g. X (R1 = Ph, R2 = Me). All the other X were prepared by essentially the same procedure as method 2. 1-Alkyl(aryl)-6-alkyl-4-alkylthiopyrazolo[3,4-d]pyrimidines (XI) (R1 = 1-substituent, R2 = 6-substituent, R3 = S-substituent were prepared as follows: X (R1 = R2 = Me) (13 g.), 40 ml. 4N KOH, 18 g. MeI, and 30 ml. MeOH shaken 0.5 hr. in a separatory funnel, the contents left overnight at 40°, and the solid collected gave 12.5 g. XI (R1 = R2 = R3 = Me). X (R1 = Ph, R2 = Me) (1 g.) added to 200 ml. H2O containing 15 g. KOH and 21 g. EtI, treated with 100 ml. alc., refluxed 5 hrs., and reduced in volume, until an oily product solidified gave 3 g. XI (R1 = Ph, R2 = Me, R3 = Et). 4-Alkoxy-1-alkyl(aryl)-6-methylpyrazolo[3,4-d]pyrimidines (XII) (R1 = 1-substituent, R2 = O-substituent) were prepared as follows: IV (R1 = p-MeC6H4, R2 = Me) (5.5 g.) and 100 ml. alc. left 2 hrs. at room temperature with 2 g. Na in 70 ml. alc., heated 40 min. on the steam bath, and NaCl removed, the filtrate treated with 50 ml. H2O, and left overnight in the cold gave 3.1 g. XII (R1 = p-MeC6H4, R2 = Et). Other XII were prepared as above. The following N:CR2.N:CR3.C:C.NR1.N:CH were prepared by the above methods (R1, R2, R3, m.p., % yield, and recrystn. solvent given): H, Me, 0H, 336-8°, 73.5, AcOH; H, Me, Cl, 140° (decomposition), 70.0, C6H6; H, Me, SH, above 300°, 80, repptd.; H, Et, OH, above 300°, 82, alc., H2O; Me, Me, OH, 277-8°, 72.5, alc., H2O; Me, Me, Cl, 74°, 70.2, C7H16; Me, Me, OMe, 107.5-8.5°, 67.5, MeOH; Me, Me, SH, 264-5°, 98, repptd.; Me, Me, SMe, 74-5°, 90.2, MeOH, H2O; CH2CH2OH, Me, OH, 265-6°, 54.8, H2O; Ph, Me, Cl, 85-6°, 83.5, C7H16; Ph, Me, SH, 268.5°, 83.3, repptd.; Ph, Me, OMe, 121.5-2.0°, -, MeOH; Ph, Me, OEt, 95-5.5°, -, alc.; Ph, Me, SMe, 135-7°, -, MeOH, H2O; Ph, Me, SEt, 86-8°, -, alc., H2O; Ph, Et, OH, 295°, 88.5, alc., H2O; Ph, Et, SH, 248-9°, 91.6, repptd.; p-MeC6H4, Me, OH, 298-300°, 93.6, alc., H2O; p-MeC6H4, Me, Cl, 89-91°, 78.1, C7H16; p-MeC6H4, Me, OMe, 121-2°, 81.2, MeOH; p-MeC6H4, Me, OEt, 93-4°, 53, alc.; o-ClC6H4, Me, Cl, 121°, 77.8, C6H14; p-BrC6H4, Me, OH, above 315°, 86.6, alc., H2O; p-BrC6H4, Me, Cl, 130.5-31°, 88.7, C6H14; p-ClC6H4, Me, OH, above 310°, 94.5, alc., H2O; p-ClC6H4, Me, Cl, 129°, 82.6, C7H16; p-ClC6H4, Me, SH, above 305°, 75.2, repptd.; p-O2NC6H4, Me, OH, above 310°, 90, repptd.; p-O2NC6H4, Me, Cl, 184°, 82, PhMe. V were prepared by the following methods: (method A) IV (R1 = H, R2 = Me) (10 g.) and 120 ml. alc. NH3 heated 8 hrs. in a bomb at 160°, the product evaporated to dryness, the residue refluxed with dilute HCl, the solution treated with C,

filtered, and the product repptd. with NH4OH, filtered, and recrystd. gave 6.5 g. V (R1 = R4 = R5 = H, R2 = Me); (method B) the above IV (5 g.) added to 7 g. BuNH2, and 120 ml. alc. and the mixture refluxed 7 hrs. gave 3 g. V (R1 = R4 = H, R2 = Me, R5 = Bu). IV (R1 = Ph, R2 = Me) (5 g.) refluxed 40 min. with 8 g. p-ClC6H4NH2 and 75 ml. alc. and the mixture filtered after cooling 3 hrs. in an ice bath gave 6.2 g. crude V (R1 = Ph, R2 = Me, R4 = H, R5 = p-ClC6H4). IV (R1 = p-ClC6H4, R2 = Me) (9 g.) refluxed on a steam bath to near dryness with 160 ml. alc. containing 10 g. PhCH2CH2NH2 and the residue added to MeOH gave 11 g. V (R1 = p-ClC6H4, R2 = Me, R4 = H, R5 = CH2CH2Ph); (method C) IV (R1 = R2 = Me) (5.5. g.), 5.5 g. furfurylamine, and 200 ml. alc. heated 8 hrs. on a steam bath, then evaporated, the residue stirred with 30 ml. 10% KOH, the alkaline solution decanted, the sirup refluxed 2 hrs. with 100 ml. C6H6, and the solution, filtered and evaporated to dryness gave 4 g. V (R1 = R2 = Me, R4 = H, R5 = furfuryl as white needles. IV (R1 = Ph, R2 = Et) (13 g.) in 150 ml. alc. treated slowly with 13 g. PhCH2NH2 in 50 ml. alc., the mixture refluxed 12 hrs., the solvent removed, and the product treated with C6H6 and several drops MeOH, and refrigerated gave 8 g. V (R1 = Ph, R2 = Et, R4 = H, R5 = CH2Ph). The following V were prepared by these methods (R1, R2, R4, R5, m.p., method of preparation, % yield, and recrystn. solvents given): H, Me, H, H, above 300°, A, 73, alc., H2O; H, Me, H, Me, above 300°, B ,60, alc., H2O; H, Me, H, Et, 273-4°, B, 56, alc.; H, Me, H, Pr, 220-2°, B, 49.1, alc.; H, Me, H, CH2Ph, 241°, B, 87.2, alc.; H, Me, H, furfuryl, 243-4°, C, 59, alc.; Me, Me, H, H, 251-2°, A, 90, alc., H2O; Me, Me, H, Me, 136-8°, B, 77.2, H2O; Me, Me, H, Et, 131.5-2.0°, C, 66.9, PhMe, C7H16; Me, Me, H, CH2Ph, 180-2°, B, 83, alc.; Me, Me, H, furfuryl, 140-1.5°, C, 54.6, alc.; Me, Me, H, o-ClC6H4, 223.5-4.0°, B, 60, alc.; Me, Me, H, p-ClC6H4, 231.5°, B, 67, alc., H2O; Me, Me, H, p-MeC6H4, 224-5.5°, B, 60, alc.; Me, Me, H, p-MeC6H4, 225-7°, B, 74.7, alc.; Me, Me, H, 2,6-Et2C6H3, 218-18.5°, B, 48.5, alc.; Me, Me, H, NH2, 259-60°, B, 87.3, alc.; Ph, Me, H, H, 287-9°, A 82.5, alc., H2O; Ph, Me, H, Me, 162-3°, B, 80.2, alc., H2O Ph, Me, Me, Me, 117-17.5°, C, 82.5, alc.; Ph, Me, H, Et, 86°, B, 87.2, alc.; Ph, Me, Et, Et, 66-8°, C, 83, alc.; Ph, Me, H, iso-Pr 143-4°, B 86, alc., H2O; Ph, Me, H, tert-Bu, 175-7°, C, 61, alc., H2O; Ph, Me, H, CH2CH2NEt2, 159-60°, C, 49.1, C7H16; Ph, Me, CH2Ph, H, 187-8°, B, 92, alc.; Ph, Me, H, furfuryl, 153-4.5°, C, 56.2, PhMe, C7H16; Ph, Me, H, Ph, 262-3°, B, 50.5, EtOCH2CH2OH; Ph, Me, H, m-BrC6H4, 215-17°, B, 68, alc.; Ph, Me, H, o-ClC6H4, 175-6°, B, 51.3, alc.; Ph, Me, H, m-ClC6H4, 192-3°, B, 90, alc.; Ph, Me, H, p-ClC6H4, 226-6.5°, B, 82, alc., H2O; Ph, Me, H, 2,6-Et2C6H3, 189-90°, B, 71.2, alc.; Ph, Me, H, NH2, 243-4°, B, 80.1, C5H5N; Ph, Me, H, NHPh, 240-1°, B, 47.5, C5H5N; Ph, Et, Me, Me, 90.5-1.0°, B, 55.5, alc.; Ph, Et, H, tert-Bu, 148-8.5°, C 73.3, alc. (sublimed); Ph, Et, H, CH2Ph, 129-9.5°, C, 48.5, C, 48.5, C6H6, alc.; Ph, Et, H, o-ClC6H4, 168-8.5°, B, 71.5, EtOCH2CH2OH; Ph, Et, H, m-ClC6H4, 187-9°, B, 74, alc.; Ph, Et, H, p-ClC6H4, 208.5-9.5°, B, 87.8, EtOCH2CH2OH; Ph, Et, H, o-MeC6H4, 175-6°, B, 75.5, alc.; Ph, Et, H, m-MeC6H4, 169.5°, B, 58, alc.; Ph, Et, H, p-MeC6H4, 199-200°, B, 78.6, alc.; Ph, Et, H, 2,5-Cl2C6H3, 181-3°, B, 42.1, alc.; Ph, Et, H, 2,6-Et2C6H3, 191-1.5°, B, 38, alc.; Ph, Et, H, NH2, 198-9°, B, 87.5, alc.; p-MeC6H4, Me, H, H, 296.5-8.0°, A, 75.7, alc.; p-MeC6H4, Me,

H, Me, 181-2.5°, B, 86, MeOH, H2O; p-MeC6H4, Me, Me, Me, 149-51°, B, 82.2, alc.; p-MeC6H4, Me, H, Et, 144-6°, B, 80, alc., H2O; p-MeC6H4, Me, H, CH2CH2NEt2, 165°, C, 62.8, PhMe, C7H16; p-MeC6H4, Me, H, o-ClC6H4, 219-21°, B, 76.5, C5H5N; p-MeC6H4, Me, H, m-BrC6H4, 218-20°, B, 63.5, alc.; o-ClC6H4, Me, H, H, 294.5-9.5°, A, 71.8, alc.; o-ClC6H4, Me, Me, Me, 152-3°, C, 77.7, alc.; o-ClC6H4, Me H, o-ClC6H4, 196-8°, B, 63, alc.; p-BrC6H4, Me, Et, Et, 123-4°, B, 51.6, EtOCH2CH2OH, H2O; p-ClC6H4, Me, H, H, above 300°, A, 36, alc.; p-ClC6H4, Me, H, Me, 218-19°, B, 57.2, alc.; H2O; p-ClC6H4, Me, H, iso-PrO(CH2)3, 109-10°, B, 51.1, MeOH, H2O; p-ClC6H4, Me, (R4R5 =) (CH2)5, 127.5-8.5°, B, 61.3, alc., H2O; p-ClC6H4, Me, H, CH2Ph, 214°, B, 93.3, EtOCH2CH2OH; p-ClC6H4, Me, H, CH2CH2Ph, 175-6°, B, 60.1, alc.; p-ClC6H4, Me, H, o-ClC6H4, 221-2°, B, 62.0, C5H5N, p-ClC6H4, Me, H, m-ClC6H4, 222-3°, B, 85.5, EtOCH2CH2OH; p-ClC6H4, Me, H, p-ClC6H4, 239-9.5°, B, 88, C5H5N; p-ClC6H4, Me, H, m-BrC6H4, 230-2°, B, 74.2, C5H5N; p-ClC6H4, Me, H, 2,5-Cl2C6H3, 200°, B, 71.5, EtOCH2CH2OH; p-O2NC6H4, Me, H, Me, 248-9°, B, 69, alc.; p-O2NC6H4, Me, Me, Me, 196°, B, 51.2, alc., H2O; p-O2NC6H4, Me, H, iso-Pr, 190-2°, B, 81.1, alc.; p-O2NC6H4, Me, H, Bu, 147°, B, 66.6, alc.; p-O2NC6H4, Me, (R4R5 =) (CH2)5, 189-91°, B, 96, C5H5N; p-O2NC6H4, Me, H, CH2CH2NEt2, 145°, B, 91.7, alc., H2O; p-O2NC6H4, Me, H, o-ClC6H4, 227-8°, B, 43.2, alc.; p-O2NC6H4, Me, H, p-ClC6H4, 278°, B, 87, AcOH. The ultraviolet spectra were given for many of the compds. given above. The screening of these compds. against tumors in mice thus far has not revealed any significant antitumor agents in this series.